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Kinetics of the distribution density and entropy of an isolated system of particles in phase space

I. G. Minkevich

G. K. Skryabin Institute of Biochemistry and Physiology of Microorganisms,
FRC Pushchino Centre for Biological Research, Russian Academy of Sciences,
5 pr. Nauki, Pushchino, Moscow Region, 142290, Russia

E-mail: minkevich@pbcras.ru

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This work lies in the field of nonequilibrium statistical mechanics. It investigates the spatiotemporal behavior of isolated many-particle systems. A phenomenological model has been formulated that combines the laws of classical dynamics and random transitions between various microscopic states of the system. All processes occurring with such a system take place on a closed hypersurface in a coordinate-momentum phase space. This surface corresponds to a fixed value of energy of the system; it is designated as Surf_E. The kinetic equation for the probability density distribution of a system in a phase space, $f(\vec{x}, t)$, is reduced to a form convenient for finding solutions to this equation ($\vec{x}$ is a set of phase variables). Proof is given that the extremum of the entropy of the system, which is found by the calculus of variations, is a maximum. Near its maximum, entropy is proportional to the integral of the squared variation of $f(\vec{x}, t)$ over the entire volume of the hypersurface Surf_E. The dependence of entropy on density variation distribution $f(\vec{x}, t)$ has been found, when this variation has constant values in two subregions of the hypersurface; these values can be rather large. A kinetic equation has been formulated for the $D(\vec{x}, t)$, deviation of particle distribution density $f(\vec{x}, t)$ from its equilibrium value. Analytical solutions of this equation have been found for several variants of the dependence of the rate of random transitions on the distance between the initial and final microscopic states of the transition. If this rate does not depend on the above-mentioned distance, the initial shape of $D(\vec{x}, t)$ is maintained throughout the entire process of the exponential decay of the quantity $D(\vec{x}, t)$. The transition process is considered in a more general case, when random transitions are possible only in a limited range of distances between microstates. Then the value $D(\vec{x}, t)$ is equal to the sum of spatial modes, each of which, as the distribution density tends to the equilibrium, decays at its own rate. The higher the order of the mode, the faster it decays. Therefore, in this case, the transition process leads not only to a general decrease of $D(\vec{x}, t)$, but also to a smoothing of the $D(\vec{x}, t)$ original shape. The general dependence of the difference between the equilibrium and nonequilibrium entropy values on $D(\vec{x}, t)$ has been found.

Keywords: system of point particles, classical dynamics, microscopic state, random transitions, probability distribution density, kinetic equation, entropy, thermodynamic equilibrium, transient processes, nonequilibrium state, solutions of the kinetic equation

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МОДЕЛИ В ФИЗИКЕ И ТЕХНОЛОГИИ

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Кинетика плотности распределения и энтропии изолированной системы частиц в фазовом пространстве

И. Г. Минкевич

Институт биохимии и физиологии микроорганизмов им. Г. К. Скрябина РАН,
ФИЦ «Пущинский научный центр биологических исследований РАН»,
Россия, 142290, Московская область, г. Пущино, пр. Науки, д. 5

E-mail: minkevich@pbcras.ru

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Данная работа лежит в области неравновесной статистической механики. Она посвящена изучению пространственно-временного поведения изолированных многочастичных систем. Сформулирована феноменологическая модель, сочетающая законы классической динамики с присутствием случайных переходов между различными микроскопическими состояниями системы. Все процессы, происходящие с такой системой, имеют место на замкнутой гиперповерхности в фазовом пространстве координат-импульсов. Эта поверхность соответствует фиксированному значению энергии системы; она обозначена как $\mathrm{Surf_E}$. Кинетическое уравнение для плотности вероятностей распределения системы в фазовом пространстве $f(\vec{x}, t)$ приведено к форме, удобной для нахождения решений этого уравнения ($\vec{x}$ — совокупность фазовых переменных). Дано доказательство того, что экстремум энтропии системы, который находится методом вариационного исчисления, является максимумом. Вблизи своего максимума энтропия пропорциональна интегралу от квадрата вариации $f(\vec{x}, t)$ по всему объему гиперповерхности $\mathrm{Surf_E}$. Найдена зависимость энтропии от вариации плотности распределения $f(\vec{x}, t)$, когда эта вариация имеет постоянные значения в двух подобластях гиперповерхности, причем эти значения могут быть весьма велики. Сформулировано кинетическое уравнение для $D(\vec{x}, t)$ — отклонения плотности распределения частиц $f(\vec{x}, t)$ от ее равновесного значения. Найдены аналитические решения этого уравнения для нескольких вариантов зависимости скорости случайных переходов от расстояния между начальным и конечным микроскопическими состояниями перехода. Если эта скорость не зависит от вышеназванного расстояния, то исходная форма $D(\vec{x}, t)$ сохраняется в течение всего процесса экспоненциального затухания величины $D(\vec{x}, t)$. Рассмотрен переходный процесс в более общем случае, когда случайные переходы возможны только в ограниченном диапазоне расстояний между микросостояниями. Тогда величина $D(\vec{x}, t)$ равна сумме пространственных мод, каждая из которых при стремлении плотности распределения к равновесному значению затухает со своей скоростью. Чем выше порядок моды, тем быстрее она затухает. Поэтому в данном случае переходный процесс приводит не только к общему уменьшению $D(\vec{x}, t)$, но и к сглаживанию первоначальной формы $D(\vec{x}, t)$. Найдена общая зависимость разности между равновесным и неравновесным значениями энтропии от величины $D(\vec{x}, t)$.

Ключевые слова: система точечных частиц, классическая динамика, микроскопическое состояние, случайные переходы, плотность распределения вероятностей, кинетическое уравнение, энтропия, термодинамическое равновесие, переходные процессы, неравновесное состояние, решения кинетического уравнения

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Introduction

Fundamentals of the statistical mechanics of many-particle systems, the particles of which are governed by the laws of classical dynamics, have been developed by J. C. Maxwell, J. W. Gibbs, and L. E. Boltzmann. A huge number of investigations has been done in this field. The description of their results and numerous references can be found, e. g., in [Зубарев, 1971; Климонтович, 1995; Ландау, Лифшиц, 1995; Лифшиц, Питаевский, 1979; Balescu, 1975; Hoch, 2021; Huang, 2010; Kennett, 2021; Kittel, Kroemer, 1980; Kondepudi, Prigogine, 1998; Müller-Kirsten, 2022; Nolting, 2018; Reichl, 2016; Sadovskii, 2019; Sekerka, 2015; Sethna, 2006]. The main part of these works relates to systems, which are in the state of thermodynamic equilibrium. At the same time, the transient processes in the nonequilibrium many-particle systems are much less studied. Interactions between microscopic states are considered based on atomic collisions where all physical details of these processes are taken into account [Лифшиц, Питаевский, 1979; Климонтович, 1995; Reichl, 2016]. The Boltzmann equation derived on this basis is rather difficult to study analytically. There are numerical methods for finding the solutions of the Boltzmann equation [Succi, 2001], but these methods have restricted capacities as an exploratory tool.

Analytical methods have considerable advantage as a tool for revealing the properties of an object of research when the solutions of equations describing this object are found. We are not familiar with any publications containing explicit solutions of kinetic equations describing the temporal behavior of nonequilibrium many-particle systems. Works in the field of nonequilibrium statistical thermodynamics concentrate mainly on formulating the mathematical description of nonequilibrium systems in general.

The present work is devoted to finding the solutions of the kinetic equation, which describe the establishment of equilibrium in an isolated system of many classical-mechanical particles. To do that, a notion of microscopic state of such a system is formulated, a phenomenological model of transitions between these states is developed; a variant of the kinetic equation, which allows finding its explicit solutions, is formulated. On this basis, the expressions for the entropy and for the rate of entropy change are obtained based on the mentioned model.

Kinetic equation

The subjects of this work are isolated systems, which possess continuous sets of microscopic states. It relates to systems of point particles the motion of which is governed by the laws of classical mechanics. Then, the microstates are characterized by coordinates and rates of the particles, or, which is equivalent to the said, by their coordinates and momenta. Here we accept the coordinate – momentum conception. Then every n-th particle is described by two vectors: generalized coordinates, $\vec{q}_n$, and generalized momenta, $\vec{p}_n$. In mechanics a combined description of the whole particle set is also applied [Ландау, Лифшиц, 1988; Nolting, 2018; Sadovskii, 2019], when a junction of coordinates of all particles, q_i (the components of all vectors $\vec{q}_n$ are placed in succession and numbered by a general index number, i) and a similar junction of momenta of all particles, p_i, are considered. For the analysis presented below, it is convenient to apply a column vector $\vec{x} = \begin{pmatrix}\vec{q}\\ \vec{p}\end{pmatrix}$, in which the column of all momenta, p_i (denoted as $\vec{p}$) is a continuation of the column of all coordinates, q_i (denoted as $\vec{q}$).

Any **macro**scopic state of a system corresponds to an aggregate of **micro**scopic states and is described by a distribution of probabilities of the system staying in separate microstates. This distribution is the total characteristic of the system behavior kinetics, of its evolution in time. During the consideration of the evolution of a large system, the behavior of entropy as an integral characteristic of the system spread over the microstates is of particular interest.

If a situation is assumed that randomness is present only at the initial time, the initial distribution of an isolated system over microstates and its entropy do **not change** in time [Зубарев, 1971; Климонтович, 1995]. Therefore, it is reasonable to accept the following notion of a microstate: not one point in the phase space $\vec{x} = \begin{pmatrix}\vec{q}\\ \vec{p}\end{pmatrix}$, but the whole trajectory that represents a deterministic description of the point motion in this space. Description of a physical reality requires completing this picture by introduction of randomness, viz., random transitions between the microstates. The above-mentioned notion of a microstate determines a random transition between the microstates as a skip from one trajectory to another.

Let us introduce the following denotations: N, the total number of particles in the system; $f(\vec{x}, t)$, the density of probability of the total system staying in the point $\vec{x}$ of the coordinate – momentum space at time t. Staying in the given microscopic state means location of the system at the trajectory passing through the point $\vec{x}$. Let us consider firstly the case when the particle motion is governed exclusively by the laws of classical mechanics, and after the initial time the system is not affected by randomness. Then the kinetics of $f(\vec{x}, t)$ is described by the following equation [Зубарев, 1971; Müller-Kirsten, 2022]

$$\frac{\partial f(\vec{x}, t)}{\partial t} + \mathrm{div}(\vec{v}(\vec{x}) f(\vec{x}, t)) = 0, \tag{1}$$

where the divergence is

$$\mathrm{div}(\vec{v}(\vec{x}) f(\vec{x}, t)) = \sum_{k=1}^{6N} \frac{\partial}{\partial x_k} (v_k(\vec{x}) f(\vec{x}, t)). \tag{2}$$

Here $\vec{v}$ is the vector of change rates of coordinates, q_i, and momenta, p_i (components of the vector of the system state, $\vec{x}$) according to the laws of particle dynamics. The index k denotes straight-through enumeration of the $\vec{x}$ components.

The motion of the point $\vec{x}$, representing the isolated system state, is described by Hamilton's equations [Ландау, Лифшиц, 1988]:

$$\frac{dq_i}{dt} = \frac{\partial H(\vec{q}, \vec{p})}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H(\vec{q}, \vec{p})}{\partial q_i}, \tag{3}$$

where H is Hamiltonian of the whole system. As a result of its isolation, $H(\vec{q}, \vec{p}) = E = \mathrm{const}$, where E is the total energy of the system. The quantities $\frac{dq_i}{dt}$ and $\frac{dp_i}{dt}$ are the rates v_k. Enumeration i relates to k as follows: $i = k$ at $k = 1 \div 3N$, and $i = k - 3N$ at $k = (3N + 1) \div 6N$.

Interrelation $H(\vec{q}, \vec{p}) = E = \mathrm{const}$ describes a hypersurface in the space $\vec{x} = \begin{pmatrix}\vec{q}\\ \vec{p}\end{pmatrix}$, within which all the events, related to the evolution of the considered particle system, occur. Let us denote this surface as $\mathrm{Surf_E}$. The density of probability distribution, $f(\vec{x}, t)$, is normalized as follows [Климонтович, 1995]:

$$\int\limits_{\mathrm{Surf_E}} f(\vec{x}, t)\, d\vec{x} = \int\limits_{\mathrm{Surf_E}} f(\vec{q}, \vec{p}, t)\, d\vec{q}\, d\vec{p} = 1. \tag{4}$$

The quantity $d\vec{x}$ is a product of differentials of all the vector $\vec{x}$ components. The integration is made over the whole $\mathrm{Surf_E}$ area, which is denoted below as Ω. The normalizing condition should be valid for all times t.

For further analysis, another form of Eq. (1) is more convenient. We consider here the case when there are momenta, q_i, but not particle rates are components of $\vec{x}$. In this case, according to Appendix 1, the expression for divergence has the following form:

$$\mathrm{div}(\vec{v}(\vec{x}) f(\vec{x}, t)) = \sum_{k=1}^{6N} v_k(\vec{x}) \frac{\partial f(\vec{x}, t)}{\partial x_k}.$$

Then,

$$\frac{\partial f(\vec{x},\, t)}{\partial t} + \sum_{k=1}^{6N} v_k(\vec{x}) \frac{\partial f(\vec{x},\, t)}{\partial x_k} = 0. \tag{5}$$

The expression in the left-hand side of Eq. (5) is known in hydrodynamics as a convectional derivative [Седов, 1970]. It is the total directional derivative along the trajectory; the latter is described by Eqs. (3) and passes via the point $\vec{x}$:

$$\frac{\partial f(\vec{x},\, t)}{\partial t} + \sum_{k=1}^{6N} v_k(\vec{x}) \frac{\partial f(\vec{x},\, t)}{\partial x_k} = \frac{df(\vec{x},\, t)}{dt}.$$

It should be emphasized that, as opposed to $\frac{\partial f(\vec{x},t)}{\partial t}$, the quantity $\frac{df(\vec{x},t)}{dt}$ is the **total** time derivative of f. Then Eq. (5) takes the form:

$$\frac{df(\vec{x},\, t)}{dt} = 0. \tag{6}$$

It means that at the absence of random transitions between the microscopic states the density of probability distribution of the system over the microstates is invariable in time.

Now let us introduce the effect of randomness into Eqs. (5) and (6). Denote the rate of the system skip from a microstate $\vec{\xi}$ to a microstate $\vec{x}$ as $\varphi(\vec{\xi},\, \vec{x})$. A reason of such an event may be, e. g., particle collision. In the model described here the transition $\vec{\xi} \to \vec{x}$ is considered as instantaneous. In all expressions where φ is involved, the first argument relates to an initial system state before the random transition, and the second to the final state. Then the kinetic equation, which has initially been Eq. (5), acquires the following form:

$$\frac{\partial f(\vec{x},\, t)}{\partial t} = -\sum_{k=1}^{K} \frac{\partial}{\partial x_k}(v_k(\vec{x}) f(\vec{x},\, t)) + \int\limits_{\mathrm{Surf_E}} \varphi(\vec{\xi},\, \vec{x}) f(\vec{\xi},\, t)\, d\vec{\xi} - f(\vec{x},\, t) \int\limits_{\mathrm{Surf_E}} \varphi(\vec{x},\, \vec{\xi})\, d\vec{\xi}. \tag{7}$$

Here the term with $\varphi(\vec{\xi},\, \vec{x})$ describes random arrival from various states $\vec{\xi}$ to the state $\vec{x}$, and the term $\varphi(\vec{x},\, \vec{\xi})$, on the contrary, describes random departure from $\vec{x}$ to other states $\vec{\xi}$. Both terms contain the same function φ, since these terms describe the same process determined on the same set of the system states. The microstates described by vectors $\vec{\xi}$ differ from those described by vectors $\vec{x}$, but $\vec{x}$ and all $\vec{\xi}$'s relate to the same time instant.

The kinetic equation Eq. (6), when random transitions between microstates are present, acquires the following form, which is convenient for its analysis:

$$\frac{df(\vec{x},\, t)}{dt} = \int\limits_{\mathrm{Surf_E}} \varphi(\vec{\xi},\, \vec{x}) f(\vec{\xi},\, t)\, d\vec{\xi} - f(\vec{x},\, t) \int\limits_{\mathrm{Surf_E}} \varphi(\vec{x},\, \vec{\xi})\, d\vec{\xi}. \tag{8}$$

Equation (8) is derived from Eq. (7) similar to the transformation from Eq. (5) to Eq. (6). It describes the evolution of the distribution density f along the trajectory $\vec{x}(t)$. The latter is described by the dynamics of the particle system in the case when the random transitions between the trajectories are absent.

The kinetic equation in the form of Eq. (8) is the most suitable for finding solutions describing transient processes in the considered systems.

Entropy

The entropy of a system, which has a continuous set of microscopic states, is as follows [Зубарев, 1971; Климонтович, 1995]

$$S = -\int\limits_{\mathrm{Surf_E}} f(\vec{q},\,\vec{p})\ln f(\vec{q},\,\vec{p})\,d\vec{q}\,d\vec{p} = -\int\limits_{\mathrm{Surf_E}} f(\vec{x})\ln f(\vec{x})\,d\vec{x}. \tag{9}$$

It is the expression for dimensionless entropy. The dimensional entropy is obtained by multiplication of S by the Boltzmann constant $k_{\mathrm{B}} = 1.38 \cdot 10^{-23}$ J/K.

Entropy is not a random quantity. The random ones are the variables $\vec{q}$ and $\vec{p}$ as well as their conjunction $\vec{x}$. The entropy Eq. (9) is an integral of an expression containing the density of probability distribution; in this respect it is similar to the moments of a random variable.

Consider the properties of the quantity Eq. (9).

1°. Let us find the shape of $f(\vec{x})$, which provides the maximum of S. In this case the microscopic state probability distribution is called microcanonical. The maximality of entropy in the case, when an isolated system comes to the state of global equilibrium, is often postulated or derived not quite strictly. The shape of the equilibrium distribution, its stability, and the entropy maximality are different but closely coupled aspects of this problem.

The condition of S extremum (maximum or minimum) is the of entropy variation to zero. At that, the variations of $\vec{x}$ (i. e., of $\vec{q}$ and $\vec{p}$) should fit two restrictions: maintenance of the normalizing condition Eq. (4) and belonging of all the considered points $\vec{x}$ to the hypersurface $\mathrm{Surf_E}$ ($H(\vec{q},\,\vec{p}) = E$). Therefore, it is necessary to find the shape of the distribution $f(\vec{q},\,\vec{p})$, which provides an extremum of the following quantity [Эльсгольц, 1965]:

$$S^* = -\int\limits_{\mathrm{Surf_E}} [f(\vec{q},\,\vec{p})\ln f(\vec{q},\,\vec{p}) - \lambda_1 f(\vec{q},\,\vec{p}) - \lambda_2(H(\vec{q},\,\vec{p}) - E)]\,d\vec{q}\,d\vec{p}, \tag{10}$$

where λ_1 and λ_2 are undetermined multipliers. As distinct from Eq. (10), similar expressions present in literature either omit the condition $H(\vec{q},\,\vec{p}) = E$ or refer it to systems, which are not isolated.

Let us denote the probability density distribution, which provides the entropy extremum, as f_{ext}. The function $f_{\mathrm{ext}}(\vec{q},\,\vec{p})$ can be found from the equality of S^* variation to zero. According to that stated in Appendix 2, it takes place when $f_{\mathrm{ext}}(\vec{q},\,\vec{p}) = \mathrm{const}$. Using the normalizing condition Eq. (4), we obtain:

$$f_{\mathrm{ext}}(\vec{q},\,\vec{p}) = \frac{1}{\Omega}. \tag{11}$$

The extremal entropy value, corresponding to this probability distribution, is

$$S_{\mathrm{ext}} = -\int\limits_{\mathrm{Surf_E}} \frac{1}{\Omega}\ln\frac{1}{\Omega}\,d\vec{q}\,d\vec{p} = \ln\Omega. \tag{12}$$

2°. During the search of entropy maximum, researchers, as a rule, confine to the variational algorithm, which provides only the conditions of the extremum. It is necessary to prove that this extremum is a maximum. To do that, let us consider entropy changes in the neighborhood of f_{ext}. As a result of all q_i and p_i variations, the probability density acquires deviation from f_{ext}: $f(\vec{q},\,\vec{p}) = \frac{1}{\Omega} + \delta f(\vec{q},\,\vec{p})$. Besides, every variation δf is not completely arbitrary: $f(\vec{q},\,\vec{p})$ should fit the normalizing condition, from which

$$\int\limits_{\mathrm{Surf_E}} \delta f(\vec{q},\,\vec{p})\,d\vec{q}\,d\vec{p} = 0. \tag{13}$$

Entropy in the neighborhood of the extremum:

$$S_{\text{ext}} + \delta S = -\int\limits_{\text{Surf}_\text{E}} \left(\frac{1}{\Omega} + \delta f\right) \ln\left(\frac{1}{\Omega} + \delta f\right) d\vec{q}\, d\vec{p}.$$

Further we use the function $y = x \ln x$ expansion into a series in the neighborhood of a point x_0 including the quadratic term:

$$x \ln x = x_0 \ln x_0 + (\ln x_0 + 1)(x - x_0) + \frac{1}{2x_0}(x - x_0)^2 + \ldots \tag{14}$$

Assuming $x_0 = \frac{1}{\Omega}$, $x - x_0 = \delta f$, we find:

$$S_{\text{ext}} + \delta S = -\int\limits_{\text{Surf}_\text{E}} \frac{1}{\Omega} \ln \frac{1}{\Omega} d\vec{x} - \left(\ln \frac{1}{\Omega} + 1\right) \int\limits_{\text{Surf}_\text{E}} (\delta f)\, d\vec{q}\, d\vec{p} - \frac{\Omega}{2} \int\limits_{\text{Surf}_\text{E}} (\delta f)^2\, d\vec{q}\, d\vec{p} + \ldots$$

Since the first term in the right-hand side is S_{ext} and the second one equals zero according to Eq. (13),

$$\delta S = -\frac{\Omega}{2} \int\limits_{\text{Surf}_\text{E}} (\delta f)^2\, d\vec{q}\, d\vec{p}. \tag{15}$$

It is seen from here that $\delta S < 0$ and, therefore, the entropy value Eq. (12) is a maximum.

3°. Let us consider the behavior of entropy within a sufficiently large range of $f(\vec{q}, \vec{p})$ deviation from $\frac{1}{\Omega}$, using the approach, which we have applied in the case of a discrete set of microscopic states [Minkevich, 2023]. Here we subdivide the surface Surf_E into two arbitrary fragments, Surf_E^1 and Surf_E^2, the areas of which are, correspondingly, Ω_1 and Ω_2, where $\Omega_1 + \Omega_2 = \Omega$. Let the probability density $f(\vec{q}, \vec{p})$ be equal to constants different from $\frac{1}{\Omega}$ within every of the above mentioned fragments. Then, $f_1 = \frac{1}{\Omega} + \delta f_1$, $f_2 = \frac{1}{\Omega} + \delta f_2$, where indices 1 and 2 denote the quantities related to Surf_E^1 and Surf_E^2, correspondingly. The normalizing condition for the probability distribution density in this case is as follows:

$$\int\limits_{\text{Surf}_\text{E}^1} f_1\, d\vec{q}\, d\vec{p} + \int\limits_{\text{Surf}_\text{E}^2} f_2\, d\vec{q}\, d\vec{p} = 1,$$

from which $\Omega_1\, \delta f_1 + \Omega_2\, \delta f_2 = 0$. The latter interrelation results in a rigid constraint on δf_1 and δf_2: $\delta f_2 = -\frac{\Omega_1}{\Omega_2}\, \delta f_1$.

Introduce parameters κ_1 and ρ_1 according to the following interrelations: $\delta f_1 = \frac{1}{\Omega}\kappa_1$, $\Omega_1 = \rho_1 \Omega$. Then, $\Omega_2 = (1 - \rho_1)\Omega$, $\delta f_2 = -\frac{\rho_1}{1-\rho_1}\frac{1}{\Omega}\kappa_1$.

In this case, entropy of the system equals

$$S = \ln \Omega + \delta S = -\int\limits_{\text{Surf}_\text{E}^1} \left(\frac{1}{\Omega} + \delta f_1\right) \ln\left(\frac{1}{\Omega} + \delta f_1\right) d\vec{q}\, d\vec{p} - \int\limits_{\text{Surf}_\text{E}^2} \left(\frac{1}{\Omega} + \delta f_2\right) \ln\left(\frac{1}{\Omega} + \delta f_2\right) d\vec{q}\, d\vec{p}. \tag{16}$$

Transforms described in Appendix 3 result in:

$$\delta S = -\rho_1(1 + \kappa_1) \ln(1 + \kappa_1) - (1 - \rho_1)\left(1 + \frac{\rho_1}{1 - \rho_1}\kappa_1\right) \ln\left(1 + \frac{\rho_1}{1 - \rho_1}\kappa_1\right). \tag{17}$$

This expression is obtained here for systems the microscopic state set of which is continuous. It is identical to that obtained in our earlier work [Minkevich, 2023] for systems with a discrete set of microstates. Correspondingly, the analysis of this expression made in the mentioned work is valid for the systems considered here.

Kinetics of particle probability distribution in phase space

1°. Let us examine the validity of the normalizing condition Eq. (4) for solutions of Eq. (8). To do that, integrate Eq. (8) over all the components of the vector $\vec{x} = \begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix}$ within the surface Surf_E:

$$\frac{d}{dt} \int\limits_{\mathrm{Surf}_\mathrm{E}} f(\vec{x},\, t)\, d\vec{x} = \int\limits_{\mathrm{Surf}_\mathrm{E}} \int\limits_{\mathrm{Surf}_\mathrm{E}} \varphi(\vec{\xi},\, \vec{x}) f(\vec{\xi},\, t)\, d\vec{\xi}\, d\vec{x} - \int\limits_{\mathrm{Surf}_\mathrm{E}} \int\limits_{\mathrm{Surf}_\mathrm{E}} f(\vec{x},\, t) \varphi(\vec{x},\, \vec{\xi})\, d\vec{\xi}\, d\vec{x}. \tag{18}$$

Both summands in the right-hand side of this expression, during the double integration, include all the possible transitions between the microstates. Redesignating the variables in the second integral ($\vec{x} \to \vec{\xi}$ and $\vec{\xi} \to \vec{x}$), we obtain that the second integral in Eq. (18) equals the first one, i. e., the rates of transitions into any state and from it compensate each other on the whole balance. Hence,

$$\frac{d}{dt} \int\limits_{\mathrm{Surf}_\mathrm{E}} f(\vec{x},\, t)\, d\vec{x} = 0 \tag{19}$$

and

$$\int\limits_{\mathrm{Surf}_\mathrm{E}} f(\vec{x},\, t)\, d\vec{x} = \mathrm{const}$$

at any time. Since const = 1 at $t = 0$, the condition of Eq. (4) is always valid. In particular, this fact confirms the correctness of the kinetic equation in the form of Eqs. (7) and (8).

2°. The stationary density for the particle distribution is $f(\vec{x}) = f_0 = \mathrm{const}$. It satisfies Eqs. (18) and (19). Substituting $f(\vec{x}) = f_0$ into Eq. (8), we obtain the rate balance:

$$\int\limits_{\mathrm{Surf}_\mathrm{E}} [\varphi(\vec{\xi},\, \vec{x}) - \varphi(\vec{x},\, \vec{\xi})]\, d\vec{\xi} = 0. \tag{20}$$

Further, substituting f_0 into the normalizing condition Eq. (4), we obtain: $f_0 = \frac{1}{\Omega}$, where $\Omega = \int\limits_{\mathrm{Surf}_\mathrm{E}} d\vec{x}$ is the area of the multidimensional surface Surf_E, within which all the events, related to the evolution of the considered particle system, occur. Hence, the stationary distribution is uniform. It coincides with f_{ext}.

3°. To study transient processes in the considered systems, let us introduce a quantity $D(\vec{x},\, t)$, which is the deviation of $f(\vec{x},\, t)$ from the stationary solution, $\frac{1}{\Omega}$:

$$f(\vec{x},\, t) = \frac{1}{\Omega} + D(\vec{x},\, t). \tag{21}$$

The normalizing condition for $D(\vec{x},\, t)$, which is the consequence of Eqs. (4) and (21), is as follows:

$$\int\limits_{\mathrm{Surf}_\mathrm{E}} D(\vec{x},\, t)\, d\vec{x} = 0. \tag{22}$$

Substituting Eq. (21) into Eqs. (7) and (8), we obtain two forms of the equation for $D(\vec{x},\, t)$:

$$\frac{\partial D(\vec{x},\, t)}{\partial t} = -\sum_{k=1}^{K} \frac{\partial}{\partial x_k} (v_k(\vec{x}) D(\vec{x},\, t)) + \int\limits_{\mathrm{Surf}_\mathrm{E}} \varphi(\vec{\xi},\, \vec{x}) D(\vec{\xi},\, t)\, d\vec{\xi} - D(\vec{x},\, t) \int\limits_{\mathrm{Surf}_\mathrm{E}} \varphi(\vec{x},\, \vec{\xi})\, d\vec{\xi}, \tag{23}$$

$$\frac{dD(\vec{x}(t),\, t)}{dt} = \int\limits_{\mathrm{Surf}_\mathrm{E}} \varphi(\vec{\xi},\, \vec{x}) D(\vec{\xi},\, t)\, d\vec{\xi} - D(\vec{x},\, t) \int\limits_{\mathrm{Surf}_\mathrm{E}} \varphi(\vec{x},\, \vec{\xi})\, d\vec{\xi}. \tag{24}$$

When considering transients, it is convenient to represent $\varphi(\vec{x}, \vec{\xi})$ in the following form:

$$\varphi(\vec{x}, \vec{\xi}) = \varphi_0 \Omega g(\vec{x}, \vec{\xi}),$$

where

$$\int\limits_{\mathrm{Surf_E}} g(\vec{x}, \vec{\xi})\, d\vec{\xi} = 1$$

for all $\vec{x}$. Then,

$$\int\limits_{\mathrm{Surf_E}} \varphi(\vec{x}, \vec{\xi})\, d\vec{\xi} = \int\limits_{\mathrm{Surf_E}} \varphi_0 \Omega g(\vec{x}, \vec{\xi})\, d\vec{\xi} = \varphi_0 \Omega.$$

The coefficient φ_0 is responsible for the intensity of random transitions between the microstates. Then Eqs. (23) and (24) take the form:

$$\frac{\partial D(\vec{x}, t)}{\partial t} = -\sum_{k=1}^{K} \frac{\partial}{\partial x_k}(v_k(\vec{x}) D(\vec{x}, t)) + \varphi_0 \Omega \int\limits_{\mathrm{Surf_E}} g(\vec{\xi}, \vec{x}) D(\vec{\xi}, t)\, d\vec{\xi} - \varphi_0 \Omega D(\vec{x}, t), \tag{25}$$

$$\frac{dD(\vec{x}, t)}{dt} = \varphi_0 \Omega \int\limits_{\mathrm{Surf_E}} g(\vec{\xi}, \vec{x}) D(\vec{\xi}, t)\, d\vec{\xi} - \varphi_0 \Omega D(\vec{x}, t). \tag{26}$$

4°. Let us consider an extreme case when $g(\vec{x}, \vec{\xi}) = \mathrm{const} = \frac{1}{\Omega}$ from which $\varphi = \varphi_0 = \mathrm{const}$. From the physical viewpoint it is difficult to imagine an object the particles of which interact at quite different distances with equal probability. But from the mathematical viewpoint this example is helpful for investigation of the behavior of the particle probability distribution density in phase space. In this case, the first term of the right-hand side of Eq. (26), according to Eq. (22), equals zero, and the equation of $D(\vec{x}, t)$ kinetics is as follows:

$$\frac{dD(\vec{x}, t)}{dt} = -\varphi_0 \Omega D(\vec{x}, t). \tag{27}$$

The solution of this equation:

$$D(\vec{x}, t) = D(\vec{x}, 0) e^{-\varphi_0 \Omega t}. \tag{28}$$

The distribution density of particles in the phase space in this case is as follows:

$$f(\vec{x}, t) = \frac{1}{\Omega} + \left[f(\vec{x}, 0) - \frac{1}{\Omega} \right] e^{-\varphi_0 \Omega t}. \tag{29}$$

It is seen from here that at $\varphi = \varphi_0$ the stationary solution $f = \frac{1}{\Omega}$ is stable since all the trajectories $\vec{x}(t)$ converge to it. At that, the form of $D(\vec{x}, t)$ $\left(\text{deviation from } f = \frac{1}{\Omega}\right)$ is invariable and the size of $D(\vec{x}, t)$ diminishes with the coefficient:

$$\frac{D(\vec{x}(t), t)}{D(\vec{x}(0), 0)} = e^{-\varphi_0 \Omega t}.$$

An extreme case, which is opposite to the one considered above, takes place when transitions between the microstates are absent at all. Then $g(\vec{x}, \vec{\xi}) = \delta(\vec{\xi} - \vec{x})$ (the delta function), and Eq. (8) has the following form:

$$\frac{df(\vec{x}(t), t)}{dt} = \varphi_0 \Omega f(\vec{x}, t) - \varphi_0 \Omega f(\vec{x}, t) = 0.$$

It is a hydrodynamic situation.

5°. Consider an intermediate situation, which is more realistic from the physical viewpoint. Let the random transitions between microscopic states occur with different probability which depends on the distance between them. We accept the following model:

$$g(\vec{\xi},\, \vec{x}) = \prod_{k=1}^{6N} g_k(\xi_k,\, x_k),$$

where each function $g_k(\xi_k,\, x_k) = g_k(\xi_k - x_k) = g_k(x_k - \xi_k)$ is symmetric about x_k. All g_k's fit the condition

$$\oint g_k(\xi_k,\, x_k)\, d\xi_k = 1,$$

which provides validity of the condition

$$\int\limits_{\mathrm{Surf_E}} g(\vec{x},\, \vec{\xi})\, d\vec{\xi} = 1.$$

Here and further each integral $\oint \ldots d\xi_i$ means the integration along one variable ξ_k at other phase variables constant. Since the integration path passes within the closed surface $\mathrm{Surf_E}$, this path is a closed line.

Further we consider a deviation from the stationary solution in the following form:

$$D(\vec{x},\, t) = \sum_{k=1}^{6N} D_k(x_k,\, t).$$

Substituting this expression into Eq. (26), we obtain for every summand D_k a separate kinetic equation, which is similar to Eq. (26):

$$\frac{dD_k(x_k,\, t)}{dt} = \varphi_0 \Omega \int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x}) D_k(\xi_k,\, t)\, d\vec{\xi} - \varphi_0 \Omega D_k(x_k,\, t).$$

Substituting the expression

$$g(\vec{\xi},\, \vec{x}) = \prod_{k=1}^{6N} g_k(\xi_k,\, x_k)$$

into this equation allows transforming the integral in its right-hand side. We use here the fact that a multiple integral from a product of one-argument functions equals the product of single integrals from each of these functions. Then

$$\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x}) D_k(\xi_k,\, t)\, d\vec{\xi} = \int\limits_{\mathrm{Surf_E}} \prod_{l=1}^{6N} g_l(\xi_l,\, x_l) D_k(\xi_k,\, t)\, d\vec{\xi} = \prod_{l=1}^{6N} \oint g_l(\xi_l,\, x_l) D_k(\xi_k,\, t)\, d\xi_k =$$

$$= \oint D_k(\xi_k,\, t) g_k(\xi_k,\, x_k)\, d\xi_k \cdot \prod_{l \neq k} \oint g_l(\xi_l,\, x_l)\, d\xi_l.$$

Since all $\oint g_l(\xi_l,\, x_l)\, d\xi_l = 1$, we obtain:

$$\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x}) D_k(\xi_k,\, t)\, d\vec{\xi} = \oint g_k(\xi_k,\, x_k) D_k(\xi_k,\, t)\, d\xi_k.$$

The surface $\mathrm{Surf_E}$ is closed, due to which the variation of any variable can occur within a restricted interval. Let us designate the length of a k'th interval as L_k. Further we calculate every integral over a closed contour, $\oint \ldots d\xi_k$, in symmetric limits from $\xi_k = x_k - \frac{L_k}{2}$ to $\xi_k = x_k + \frac{L_k}{2}$. Then the kinetic equations for $D_k(x_k)$ in the present model have the form:

$$\frac{dD_k(x_k,\, t)}{dt} = \varphi_0\Omega \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k,\, x_k) D_k(\xi_k)\, d\xi_k - \varphi_0\Omega D_k(x_k,\, t). \tag{30}$$

We remind that k is the number of a variable from the phase space.

A solution for each function $D_k(x_k,\, t)$ is here searched for as a series:

$$D_k(x_k,\, t) = \sum_{m=1}^{\infty} D_{km}(x_k) U_{km}(t). \tag{31}$$

The form of the functions $D_{km}(x_k)$ and $U_{km}(t)$ is defined below. From (31) it follows:

$$\frac{dD_k(x_k,\, t)}{dt} = \sum_{m=1}^{\infty} D_{km}(x_k) \frac{dU_{km}(t)}{dt}. \tag{32}$$

Substituting Eqs. (31) and (32) into Eq. (30), we obtain an aggregate of equations. For every m'th summand of Eq. (31) the corresponding equation is as follows:

$$D_{km}(x_k) \frac{dU_{km}(t)}{dt} = \varphi_0\Omega \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k,\, x_k) D_{km}(x_k) U_{km}(t)\, d\xi_k - \varphi_0\Omega D_{km}(x_k) U_{km}(t).$$

Dividing every such equation by $D_{km}(x_k)U_{km}(t)$ results in separation of variables:

$$\frac{1}{U_{km}(t)} \frac{dU_{km}(t)}{dt} = \frac{1}{D_{km}(x_k)} \left[\varphi_0\Omega \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k,\, x_k) D_{km}(x_k)\, d\xi_k - \varphi_0\Omega D_{km}(x_k) \right] = -\lambda_{km}. \tag{33}$$

The minus at λ_{km}, so far an unknown quantity, is introduced for the convenience of λ_{km} utilization.

Then the equation for every $U_{km}(t)$ gets a simple form:

$$\frac{dU_{km}(t)}{dt} = -\lambda_{km} U_{km}(t). \tag{34}$$

Its solution:

$$U_{km}(t) = U_{km}(0) e^{-\lambda_{km} t}. \tag{35}$$

The value of λ_{km} will be found below.

The space-dependent part of Eq. (33) gives the following equation:

$$\varphi_0\Omega \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k,\, x_k) D_{km}(x_k)\, d\xi_k + (\lambda_{km} - \varphi_0\Omega) D_{km}(x_k) = 0. \tag{36}$$

We search for the totality of quantities $D_{km}(x_k)$ in the form of trigonometric series. Every function $D_{km}(x_k)$ is represented by the following expression:

$$D_{km}(x_k) = A_{km}\cos\left(2\pi m\frac{x_k}{L_k}\right) + B_{km}\sin\left(2\pi m\frac{x_k}{L_k}\right). \tag{37}$$

In our case, this formula is applied within the interval $0 \leqslant x_k \leqslant L_k$ for all m. The expressions of Eqs. (37) establish the form of *space modes*, forming the solution of Eq. (30). Due to the condition Eq. (22) the quantities D_{km} should not have a constant component (independent of x_k). Therefore, the numbers of modes m lie in the range $1 \leqslant m < \infty$.

Taking into account that any function g_k should be symmetric and, correspondingly, have the form $g_k(\xi_k, x_k) = g_k(\xi_k - x_k) = g_k(x_k - \xi_k)$ (see above), the integral in Eq. (36) equals to

$$\int\limits_{x_k-L_k/2}^{x_k+L_k/2} g_k(\xi_k - x_k)D_{km}(x_k)\,d\xi_k =$$

$$= A_{km}\int\limits_{x_k-L_k/2}^{x_k+L_k/2} g_k(\xi_k - x_k)\cos\left(2\pi m\frac{x_k}{L_k}\right)d\xi_k + B_{km}\int\limits_{x_k-L_k/2}^{x_k+L_k/2} g_k(\xi_k - x_k)\sin\left(2\pi m\frac{x_k}{L_k}\right)d\xi_k. \tag{38}$$

Transformation of this equality is given in Appendix 4. Substituting its result, Eq. (55), into Eq. (36), we obtain:

$$\left[\varphi_0\Omega\int\limits_{x_k-L_k/2}^{x_k+L_k/2} g_k(\xi_k - x_k)\cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right)d\xi_k + (\lambda_{km} - \varphi_0\Omega)\right]D_{km}(x_k) = 0.$$

Since we are searching for a nonzero $D_{km}(x_k)$ solution, this equation means the equality to zero of the expression in square brackets. The latter brings for the following λ_{km} solution, which is valid for any symmetric (and, certainly, nonnegative) function $g_k(\xi_k - x_k)$:

$$\lambda_{km} = \varphi_0\Omega(1 - I_{km}), \tag{39}$$

where

$$I_{km} = \int\limits_{x_k-L/2}^{x_k+L/2} g_k(\xi_k - x_k)\cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right)d\xi_k. \tag{40}$$

Since the integrand in Eq. (40) is symmetric about the argument $\xi_k - x_k$ and the integral is taken within symmetric limits, the following expression for I_{km}, suitable for numeric studies, is also valid:

$$I_{km} = 2\int\limits_{x_k}^{x_k+L/2} g_k(\xi_k - x_k)\cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right)d\xi_k. \tag{41}$$

Recall that D_k is a deviation (along the k'th phase coordinate) of the distribution density from its stationary value. The λ_{km} describes the damping rate of the D_k m'th mode.

6°. Of interest is to what extent the damping coefficient of every m'th mode, λ_{km}, depends on the form of $g_k(\xi_k - x_k)$. Since the function g_k describes the probability of transition between microscopic

states, an important characteristic of its form is $\sigma^2_{\xi_k}$, the dispersion of random variable $\xi_k - x_k$. The larger $\sigma^2_{\xi_k}$ is, the farther from each other the microscopic states (dynamic trajectories), between which the random transition is possible, are. The dependence of λ_{km} on $\sigma^2_{\xi_k}$ is suitable for comparison of various $g_k(\xi_k - x_k)$ from the viewpoint of the influence of the form of this function on the mode damping rate.

Let us consider first the behavior of $\lambda_{km}\left(\sigma^2_{\xi_k}\right)$ near $\sigma^2_{\xi_k} = 0$. Represent the cosine in the neighborhood of the point $\xi_k = x_k$ as a sum of the first two terms of the Taylor series expansion:

$$\cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right) = 1 - \frac{1}{2}\left(2\pi m\frac{\xi_k - x_k}{L_k}\right)^2.$$

It can be seen from here that in the neighborhood of the point $\xi_k = x_k$ the cosine is close to a parabola the branches of which are directed down and go the steeper the larger the mode number m is. Further, when ξ_k is moving away from x_k, the functions $g_k(\xi_k - x_k)$ are diminishing and tend to zero at a sufficiently large distance of ξ_k from x_k. We choose the range of $|\xi_k - x_k| \leqslant \varsigma_k$ values which excludes "tails" of the function $g_k(\xi_k - x_k)$ so that the integral $\int\limits_{x_k-\varsigma_k}^{x_k+\varsigma_k} g_k(\xi_k - x_k)\,d\xi_k$ remains close to unity. It corresponds to the g_k normalizing condition. Consider those m values at which the $\cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right)$, being in the argument range $|\xi_k - x_k| \leqslant \varsigma_k$, can be represented as the above-mentioned parabola. Then:

$$I_{km} = \int\limits_{x_k-L/2}^{x_k+L/2} g_k(\xi_k - x_k)\,d\xi_k - \frac{1}{2}\left(\frac{2\pi m}{L_k}\right)^2 \int\limits_{x_k-L/2}^{x_k+L/2} (\xi_k - x_k)^2 g_k(\xi_k - x_k)\,d\xi_k = 1 - 2(\pi m)^2\frac{\sigma^2_{\xi_k}}{(L_k)^2},$$

from which

$$\lambda_{km} = 2\pi^2\varphi_0\Omega m^2\frac{\sigma^2_{\xi_k}}{(L_k)^2}. \tag{42}$$

This result does not depend on a specific form of the function $g_k(\xi_k - x_k)$. It shows that in the case when random transitions are possible only between adjacent microstates, the rates of mode damping are proportional to $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$, which is the relative dispersion of such a transition distance. These rates sharply increase as the mode number grows (proportionally to m^2).

Figure 1 shows a number of $1 - I_{km}$ dependencies on $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$ for various m values. The shape of the function $1 - I_{km}\left(\frac{\sigma^2_{\xi_k}}{(L_k)^2}\right)$ determines the form of the $\lambda_{km}\left(\frac{\sigma^2_{\xi_k}}{(L_k)^2}\right)$ dependence. The plots present in Fig. 1 are obtained by numerical integration according to an algorithm described below. As a definite $g_k(\xi_k - x_k)$ dependence, we have taken the normal (Gaussian) distribution of a random variable $(\xi_k - x_k)$. It can be seen from the figure that the initial parts of the curves adjacent to $\frac{\sigma^2_{\xi_k}}{(L_k)^2} = 0$ are rectilinear, which corresponds to the general regularity described by Eq. (42). The higher m is, the lower the $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$ values, at which the deviations of the curves from rectilinearity become appreciable, are.

The study of the dependence of $\lambda_{km}\left(\sigma^2_{\xi_k}\right)$ within a wider range of $\xi_k - x_k$ values, in which the cosine in Eqs. (40) and (41) cannot be represented as a quadratic parabola, in a general case requires numerical methods although for certain functions $g_k(\xi_k - x_k)$ the integral I_{km} can be found by quadratures.

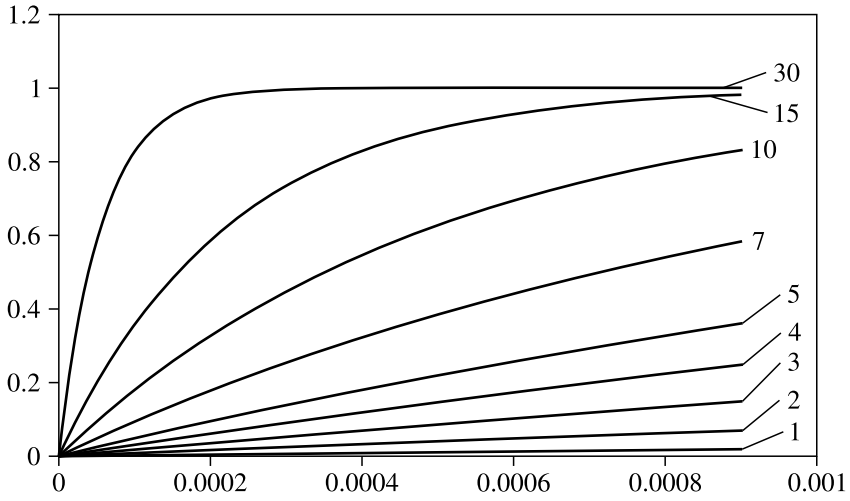


Figure 1. Dependencies of the quantity $1-I_{km}$ on relative dispersion of the distance of random transitions between microscopic states, $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$, at different values of mode order m

Let us consider dependencies $\lambda_{km}\left(\sigma^2_{\xi_k}\right)$ within the full range of variables ξ_k: $x_k - \frac{L_k}{2} \leqslant \xi_k \leqslant x_k + \frac{L_k}{2}$. It means that the "tails" of probability distributions usually determined on the infinite interval $(-\infty, +\infty)$ are truncated. The latter fact affects the normalizing factor of the function $g_k(\xi_k - x_k)$, the expression of dispersion and some other quantities. Certainly, when $g_k(\xi_k - x_k)$ is located mainly near $\xi_k = x_k$, this truncation practically does not affect the above-mentioned quantities. But when the dispersion of $\xi_k - x_k$ is not small compared with L_k, the neglect of $g_k(\xi_k - x_k)$ "tails" matters.

For numerical studies we use the representation of I_{km} in the form of Eq. (41). The functions g_k considered below depend on the argument $\frac{\xi_k - x_k}{a_k}$, where a_k is a scale parameter on which the dispersion of a random variable $(\xi_k - x_k)$ depends. Therefore, we represent g_k as

$$g_k(\xi_k, x_k) = C_k h_k\left(\frac{\xi_k - x_k}{a_k}\right),$$

where $h_k\left(\frac{\xi_k - x_k}{a_k}\right)$ defines the form of the dependence of g_k on its argument, and C_k is a normalizing factor. Then the normalizing condition,

$$\oint g_k(\xi_k, x_k)\, d\xi_k = \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k, x_k)\, d\xi_k = 1,$$

becomes as follows:

$$C_k \int\limits_{x_k}^{x_k + L_k/2} h_k\left(\frac{\xi_k - x_k}{a_k}\right) d\xi_k = \frac{1}{2},$$

from which

$$C_k = \left[2 \int\limits_{x_k}^{x_k + L_k/2} h_k\left(\frac{\xi_k - x_k}{a_k}\right) d\xi_k\right]^{-1}. \tag{43}$$

The dispersion:

$$\sigma_{\xi_k}^2 = \int\limits_{x_k - L_k/2}^{x_k + L_k/2} (\xi_k - x_k)^2 g_k(\xi_k - x_k)\, d\xi_k = 2C_k \int\limits_{x_k}^{x_k + L_k/2} (\xi_k - x_k)^2 h_k\left(\frac{\xi_k - x_k}{a_k}\right) d\xi_k. \tag{44}$$

The integral I_{km}:

$$I_{km} = 2C_k \int\limits_{x_k}^{x_k + L_k/2} h_k\left(\frac{\xi_k - x_k}{a_k}\right) \cos\left(2\pi m \frac{\xi_k - x_k}{L_k}\right) d\xi_k. \tag{45}$$

Let us introduce a dimensionless variable $y_k = \frac{\xi_k - x_k}{L_k}$. It is appropriate both for numerical calculations and for greater generality of the analysis present here since the quantities L_k in a general case have different values for different material systems. Then

$$g_k(\xi_k,\, x_k)\, d\xi_k = C_k L_k h_k\left(\frac{y_k}{\frac{a_k}{L_k}}\right) dy_k,$$

the range of integration $x_k \leqslant \xi_k \leqslant x_k + \frac{L_k}{2}$ becomes $0 \leqslant y_k \leqslant \frac{1}{2}$, the parameter a_k becomes a dimensionless parameter $\frac{a_k}{L_k}$. Correspondingly, Eqs. (43)–(45) take the following form.

The normalizing condition:

$$C_k L_k = \left[2 \int\limits_0^{1/2} h_k\left(\frac{y_k}{\frac{a_k}{L_k}}\right) dy_k\right]^{-1}. \tag{46}$$

The relative dispersion of the distance of random transitions between microstates:

$$\frac{\sigma_{\xi_k}^2}{L_k^2} = 2C_k L_k \int\limits_0^{1/2} y_k^2 h_k\left(\frac{y_k}{\frac{a_k}{L_k}}\right) dy_k. \tag{47}$$

The integral I_{km}:

$$I_{km} = 2C_k L_k \int\limits_0^{1/2} h_k\left(\frac{y_k}{\frac{a_k}{L_k}}\right) \cos(2\pi m y_k)\, dy_k. \tag{48}$$

When $h_k\left(\frac{\xi_k - x_k}{a_k}\right)$ is specified, the expressions Eqs. (46)–(48) determine the algorithm of numeric calculation of the quantity $1 - I_{km}\left(\frac{\sigma_{\xi_k}^2}{L_k^2}\right)$, which, in turn, determines the form of the dependence $\lambda_{km}\left(\frac{\sigma_{\xi_k}^2}{L_k^2}\right)$.

Let us consider the dependence $1 - I_{km}\left(\frac{\sigma_{\xi_k}^2}{L_k^2}\right)$ within the full range of the argument $\frac{\sigma_{\xi_k}^2}{L_k^2}$ for several variants of the function $g_k\left(\frac{\xi_k - x_k}{a_k}\right)$. All of them fit the normalizing condition

$$\int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k\left(\frac{\xi_k - x_k}{a_k}\right) d\xi_k = 1$$

and the requirement of symmetry

$$g_k\left(\frac{\xi_k - x_k}{a_k}\right) = g_k\left(\frac{x_k - \xi_k}{a_k}\right).$$

The most physically realistic is the normal distribution of probability of random transitions between microscopic states. Then

$$h_k = \exp\left\{-\frac{(\xi_k - x_k)^2}{2a_k^2}\right\} = \exp\left\{-\frac{y_k^2}{2\left(\frac{a_k}{L_k}\right)^2}\right\}.$$

When the normal distribution is considered on the infinite interval $(-\infty, +\infty)$, a_k^2 equals the dispersion of the random variable $\xi_k - x_k$. When $\xi_k - x_k$ is determined on the interval $\left(-\frac{L_k}{2}, \frac{L_k}{2}\right)$, the dispersion is found using Eq. (47). To calculate the dependence $1 - I_{km}\left(\frac{\sigma^2_{\xi_k}}{L_k^2}\right)$, it is necessary to obtain a sufficient number of values of $\frac{\sigma^2_{\xi_k}}{L_k^2}$ and I_{km}. It is done by running through the values of $\frac{a_k}{L_k}$ and using Eqs. (46)–(48).

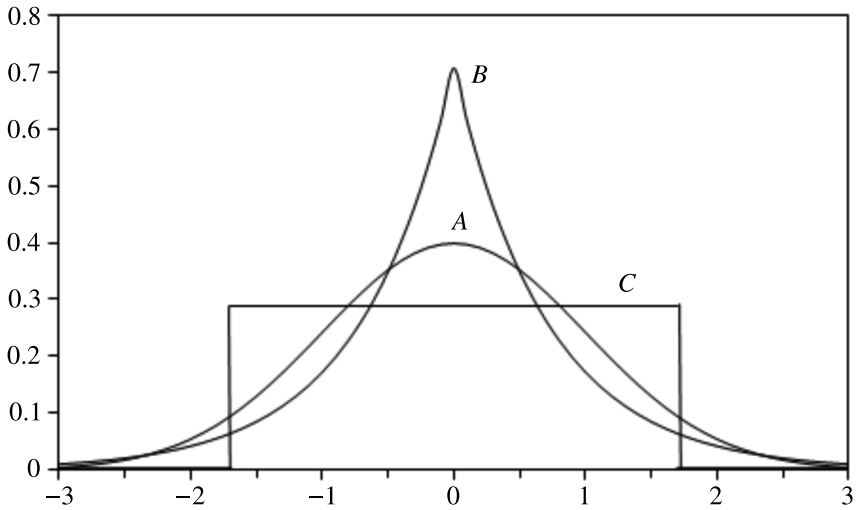


Figure 2. Shape of the distribution functions considered in the present work. *A*: normal distribution; *B*: Laplace distribution; *C*: uniform distribution

To study the influence of the form of $g_k(\xi_k - x_k)$ upon the dependence of $1 - I_{km}$ on $\frac{\sigma^2_{\xi_k}}{L_k^2}$, we have considered two more species of h_k: 1) the Laplace (or double exponential) distribution

$$h_k = \exp\left\{-\frac{|\xi_k - x_k|}{a_k}\right\} = \exp\left\{-\frac{|y_k|}{\frac{a_k}{L_k}}\right\},$$

and 2) the uniform distribution: $h_k(\xi_k - x_k) = 1$ at $x_k - \frac{a_k}{2} \leqslant \xi_k \leqslant x_k + \frac{a_k}{2}$, and $h_k(\xi_k - x_k) = 0$ outside these limits. The first has "tails", which decrease more slowly than the "tails" of the normal distribution; the second does not have "tails" at all. All the three distributions are shown in Fig. 2. All of them are built for the same dispersion value equal to unity. It is clear from the plots that distributions *B* and *C* significantly differ from the normal one. It can be seen also from the fact that the known values of

the coefficient of kurtosis are: zero for the normal distribution, 3 for the Laplace distribution, and $-\frac{6}{5}$ for the uniform distribution. The difference of the signs indicates that the differences of the shapes of distributions B and C from that of the normal distribution are opposite to one another. Therefore, comparison of the dependence $\lambda_{km}\left(\frac{\sigma^2_{\xi_k}}{(L_k)^2}\right)$ for these three distributions is informative as far as the effect of the distribution shape on the rate of the mode damping is concerned.

The dependencies of $1 - I_{km}$ on $\frac{\sigma^2_{\xi_k}}{L_k^2}$, i. e., on the relative dispersion of $(\xi_k - x_k)$ (the distance of a random transition between microstates) are present in Fig. 3. For the transitions by the laws of the normal and Laplace distributions the plots are calculated numerically as described above. For the uniform distribution the calculations are easily made analytically:

$$I_{km} = \frac{1}{a_k}\int\limits_{x_k - a_k/2}^{x_k + a_k/2} \cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right)d\xi_k = \frac{1}{a_k}\frac{L_k}{2\pi m}\sin\left(2\pi m\frac{\xi_k - x_k}{L_k}\right)\Bigg|_{\xi_k = x_k - a_k/2}^{\xi_k = x_k + a_k/2} = \frac{L_k}{a_k \pi m}\sin\left(\pi m\frac{a_k}{L_k}\right),$$

$$\lambda_{km} = \varphi_0\Omega\left[1 - \frac{1}{a_k}\frac{L_k}{\pi m}\sin\left(\pi m\frac{a_k}{L_k}\right)\right].$$

Since the uniform distribution does not have “tails”, its dispersion, as in the case when this random variable is defined in the interval $(-\infty, +\infty)$, equals to $\sigma^2_{\xi_k} = \frac{(a_k)^2}{12}$. The quantity a_k is capable of varying within the interval $0 < a_k \leqslant L_k$. At $\frac{a_k}{L_k} = 1$, the rate of transition between microstates is independent of the distance between them; this case is considered in item 4° of this section. Correspondingly, the maximal value of the relative dispersion for the uniform distribution is 0.083. To facilitate the comparison of dependencies $1 - I_{km}\left(\frac{\sigma^2_{\xi_k}}{L_k^2}\right)$ for the above-mentioned variants of $h_k\left(\frac{\xi_k - x_k}{a_k}\right)$, all the three plots in Fig. 3 are present in the same range of the argument: $0 \leqslant \frac{\sigma^2_{\xi_k}}{L_k^2} \leqslant 0.08$.

It can be seen from Fig. 3 that there are certain distinctions between the considered variants of $1 - I_{km}\left(\frac{\sigma^2_{\xi_k}}{L_k^2}\right)$ corresponding to different functions $h_k\left(\frac{\xi_k - x_k}{a_k}\right)$. But as for their principal properties, the found regularities are highly similar. At low values of $\frac{\sigma^2_{\xi_k}}{L_k^2}$ (dispersion of the distance of random transitions between the microstates) the rectilinear dependencies for the damping rate of each mode, $\lambda_{km}\left(\frac{\sigma^2_{\xi_k}}{(L_k)^2}\right)$ (at each definite value of m) coincide for all functions h_k. At higher values of $\frac{\sigma^2_{\xi_k}}{L_k^2}$, the curves rise to a plateau, the size of which is approximately the same and is close to unity for all considered variants. A markedly distinct one is only the uniform distribution, which shows a rippling of $1 - I_{km}$ for $m > 1$ during an increase of the dispersion. The reason is the interaction of the sharp edges of the uniform distribution with the cosine under the integral I_{km}. Since the uniform (Π-shaped) distribution for such kind of systems is rather a theoretical abstraction, the above-mentioned rippling may hardly be found in reality. At $m = 1$ all plots in Fig. 3 practically coincide. At higher m’s, one can see some distinctions in the trends of approaching the plateau, or (in the case of the uniform distribution) approaching the first maximum. Nevertheless, we can conclude that the species of the function $h_k\left(\frac{\xi_k - x_k}{a_k}\right)$ as a whole affect the mode damping insignificantly, and at the low range of transitions between the microstates do not affect the damping rates at all.

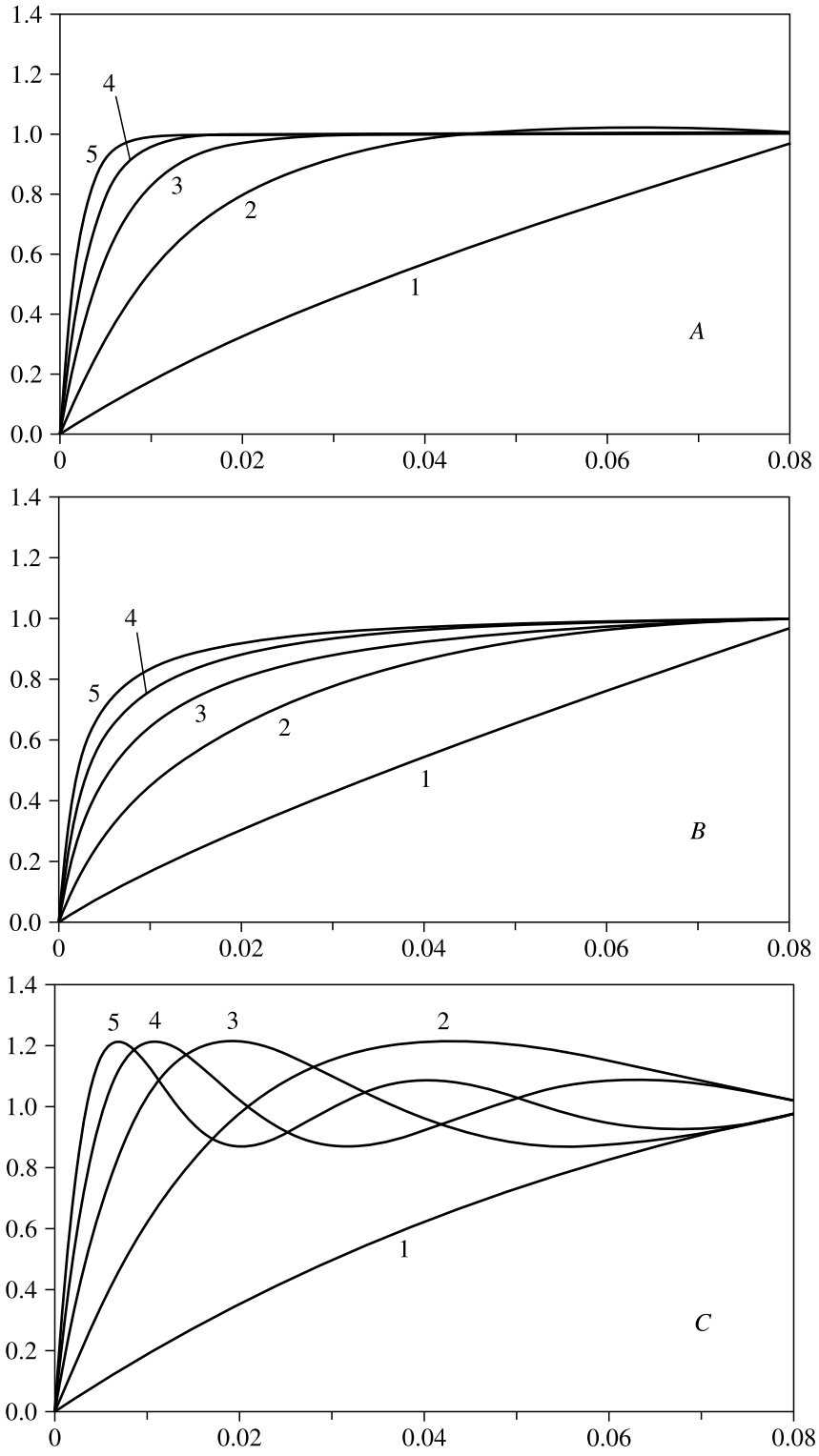


Figure 3. Dependence of the factor $1 - I_{km}$ on the relative dispersion $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$ for various functions $g_k(\xi_k - x_k)$, describing the probability distribution of random transitions between microscopic states. *A*: normal distribution; *B*: Laplace distribution; *C*: uniform distribution. Values of parameter m (the order of a mode) are shown at the corresponding curves

Expressions for entropy and the rate of its change

1°. Consider the expression for entropy (9), in which the particle distribution density is substituted by Eq. (21):

$$S(t) = -\int\limits_{\mathrm{Surf_E}} \left(\frac{1}{\Omega} + D(\vec{x},\, t)\right) \ln\left(\frac{1}{\Omega} + D(\vec{x},\, t)\right) d\vec{x}. \tag{49}$$

Using the following interrelations: $\frac{1}{\Omega} + D(\vec{x},\, t) = \frac{1}{\Omega}(1 + \Omega D(\vec{x},\, t))$, $\ln\left(\frac{1}{\Omega} + D(\vec{x},\, t)\right) = -\ln\Omega + \ln(1 + \Omega D(\vec{x},\, t))$, $\int\limits_{\mathrm{Surf_E}} d\vec{x} = \Omega$, and $\int\limits_{\mathrm{Surf_E}} D(\vec{x},\, t)\, d\vec{x} = 0$, we transform Eq. (49) as follows:

$$S(t) = \ln\Omega - \frac{1}{\Omega}\int\limits_{\mathrm{Surf_E}} (1 + \Omega D(\vec{x},\, t))[\ln(1 + \Omega D(\vec{x},\, t))]\, d\vec{x}. \tag{50}$$

The subtrahend in the right-hand side of Eq. (50) shows how much the entropy in a nonequilibrium situation is lower than its maximal value, which takes place in the case of thermodynamic equilibrium.

When deviations of $f(\vec{x},\, t)$ from $\frac{1}{\Omega}$ are small, the following inequality takes place: $\Omega D(\vec{x},\, t) \ll 1$. By decomposition of the integrand in Eq. (50), which is made based on (14), we obtain that the entropy near the stationary state of the system is as follows:

$$S(t) = \ln\Omega - \frac{\Omega}{2}\int\limits_{\mathrm{Surf_E}} [D(\vec{x},\, t)]^2\, d\vec{x}.$$

The second term in the latter expression coincides with Eq. (15). Deviation from the stationary distribution density, $D(\vec{x},\, t)$, acts as variation δf in (15).

In contrast, away from the equilibrium state ($\Omega D(\vec{x},\, t) \gg 1$), the following approximation is valid: $\ln(1 + \Omega D(\vec{x},\, t)) \approx \ln[\Omega D(\vec{x},\, t)]$. Then,

$$S(t) = \ln\Omega - \int\limits_{\mathrm{Surf_E}} D(\vec{x},\, t) \ln D(\vec{x},\, t)\, d\vec{x}.$$

In this case the following limitation on $D(\vec{x},\, t)$ values takes place:

$$\int\limits_{\mathrm{Surf_E}} D(\vec{x},\, t) \ln D(\vec{x},\, t)\, d\vec{x} \leqslant \ln\Omega$$

(entropy cannot be negative).

2°. Differentiation of Eq. (50) by time gives:

$$\frac{dS}{dt} = -\int\limits_{\mathrm{Surf_E}} \frac{dD(\vec{x},\, t)}{dt} \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x} - \int\limits_{\mathrm{Surf_E}} \frac{dD(\vec{x},\, t)}{dt} d\vec{x}.$$

Substituting $f(\vec{x},\, t) = \frac{1}{\Omega} + D(\vec{x},\, t)$ into (19), we find that the second integral in the latter equation equals zero. Then

$$\frac{dS}{dt} = -\int\limits_{\mathrm{Surf_E}} \frac{dD(\vec{x},\, t)}{dt} \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x}.$$

Substituting here $\frac{dD(\vec{x},t)}{dt}$ from (24) and using $\varphi(\vec{x},\vec{\xi}) = \varphi_0\Omega g(\vec{x},\vec{\xi})$, we find:

$$\frac{dS}{dt} = \varphi_0\Omega \int\limits_{\mathrm{Surf_E}} D(\vec{x},t)\ln(1+\Omega D(\vec{x},t))\,d\vec{x} - \varphi_0\Omega \int\limits_{\mathrm{Surf_E}} \left[\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\vec{x})D(\vec{\xi},t)\,d\vec{\xi}\right]\ln(1+\Omega D(\vec{x},t))\,d\vec{x}. \quad (51)$$

The transform of Eq. (51) is described in Appendix 5. As a result, we obtain the following expression for the rate of entropy change:

$$\frac{dS}{dt} = \varphi_0\Omega[\ln\Omega - S(t) - S_g(t)], \quad (52)$$

where

$$S_g(t) = \frac{1}{\Omega}\int\limits_{\mathrm{Surf_E}}\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\vec{x})(1+\Omega D(\vec{\xi},t))\ln(1+\Omega D(\vec{x},t))\,d\vec{\xi}d\vec{x}. \quad (53)$$

When a particle system comes to a stationary (equilibrium) state, we have the following equalities: $D(\vec{x},t) = 0$, the logarithm in the integrand is zero, $S_g = 0$, $\frac{dS}{dt} = 0$ and $S = \ln\Omega$, which confirms the correctness of Eqs. (52) and (53).

Let us find the quantity S_g when $g(\vec{\xi},\vec{x})$ has one of the extreme dependencies on its arguments. When $g(\vec{\xi},\vec{x}) = \delta(\vec{\xi}-\vec{x})$, the integral

$$\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\vec{x})(1+\Omega D(\vec{\xi},t))\,d\vec{\xi} = 1+\Omega D(\vec{x},t).$$

Then, comparing (53) with (50), we find that in this case $S_g(t) = \frac{1}{\Omega}\Omega(\ln\Omega - S(t)) = \ln\Omega - S(t)$ and, according to (52), $\frac{dS}{dt} = 0$: the entropy of the system is constant, which coincides with the previous results.

Another extreme case takes place, when $g(\vec{x},\vec{\xi}) = \mathrm{const} = \frac{1}{\Omega}$ (see above). Then, using the following equalities: $\int\limits_{\mathrm{Surf_E}} d\vec{x} = \Omega$ and $\int\limits_{\mathrm{Surf_E}} D(\vec{x},t)\,d\vec{x} = 0$, we find:

$$\frac{dS}{dt} = \varphi_0\Omega[\ln\Omega - S(t) - S_g(t)] = \varphi_0\Omega\left[\ln\Omega - S(t) - \frac{1}{\Omega}\int\limits_{\mathrm{Surf_E}}\ln(1+\Omega D(\vec{x}))\,d\vec{x}\right]. \quad (54)$$

Results and discussion

The results described above have been obtained based on the model of a many-particle object, the temporal behavior of which combines the deterministic dynamics of a mechanical system with the effect of randomness. An important property of the model is the representation of a microscopic state not as a point in a classical phase space but as a multidimensional dynamic trajectory in this space. Another important issue is application of a phenomenological dependence of the rate of random transitions between microstates, $\varphi(\vec{\xi},\vec{x})$, on the mutual location of these states. This rate is represented as a product of a coefficient dependent upon the system phase volume, Ω, on the function $g(\vec{x},\vec{\xi})$ normalized to unity. In the present work it is accepted that $g(\vec{x},\vec{\xi})$ is a product of functions $g_k(\xi_k - x_k)$ (k is a number of the phase coordinate), where each g_k depends on a single variable and is symmetric relative to its argument: $g_k(\xi_k - x_k) = g_k(x_k - \xi_k)$. In particular, it means that random transitions along individual phase coordinates are not correlated with one another. A case, when such correlation is present, is a subject of a separate study. The influence of the form of functions $g_k(\xi_k - x_k)$ on the properties of transients in nonequilibrium systems is considered in this work (see below).

Another peculiarity of the present problem is as follows: all the states of the considered system are described by points belonging to a closed hypersurface in the full phase space. It is a result of constancy of the total system energy due to its physical closure. All the events occurring with this system take place within this hypersurface. Its closure, in particular, results in the fact that each phase variable can vary within a limited interval. The full length of this interval, L_k, serves as a parameter of the mathematical description of a system kinetics.

A significant detail of the analysis described here is application of the function $D(\vec{x}, t)$, which is the deviation of the probability density of particle distribution in the phase space, $f(\vec{x}, t)$, from its stationary, i. e., equilibrium value. The latter equals $\frac{1}{\Omega}$, where Ω is the full phase volume of the above-mentioned hypersurface. The equilibrium probability distribution of the system staying in different microstates is uniform and stable. According to the normalizing condition of the probability density, the integral of $D(\vec{x}, t)$ equals zero. It means that deviations of $f(\vec{x}, t)$ from its equilibrium value should be in different directions.

We have shown that $D(\vec{x}, t)$ is the sum of deviations along separate phase coordinates:

$$D(\vec{x}, t) = \sum_{k=1}^{6N} D_k(x_k, t).$$

The kinetics of each $D_k(x_k, t)$ is considered along the phase trajectories, which considerably facilitates its analysis. It has been found that the behavior of each $D_k(x_k, t)$ is an exponential damping of the sum of spatial modes, and each m'th mode has its own damping coefficient λ_{km}.

The expression for λ_{km} includes an integral the integrand of which includes a factor $g_k(\xi_k - x_k)$. The question of interest is to what extent the value of λ_{km} depends on the form of function $g_k(\xi_k - x_k)$. We have found that the main factor affecting the value of λ_{km} is $\sigma^2_{\xi_k}$, the dispersion of the random variable $(\xi_k - x_k)$. In a number of interrelations obtained in this work the dispersion participates as a relative quantity $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$. The value of the dispersion determines the range of variable $(\xi_k - x_k)$ within which there is a real possibility of random transition into the microstate $\vec{x}$ from other microstates with coordinates $\vec{\xi}$. It has been found that at relatively small values of $\sigma^2_{\xi_k}$ (when the random transitions to a point x_k are possible from points ξ_k sufficiently close to x_k), the form of the function g_k does not affect λ_{km} at all. In this case the value of λ_{km} for any g_k is proportional to $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$.

To study the influence of the form of g_k on the coefficient of mode damping λ_{km} at high dispersion values, we have taken three variants of $g_k(\xi_k - x_k)$: 1) the normal (Gaussian) distribution as the most physically realistic species of the probability density of a continuous random variable; 2) the Laplace (double exponential) distribution; and 3) the uniform distribution. All three variants markedly differ from one another by their shape. It is shown in Fig. 2 where these distributions are given for the same value of dispersion. It is found that generally the dependence $\lambda_{km}\left(\frac{\sigma^2_{\xi_k}}{(L_k)^2}\right)$ has the following form: it is a function, which linearly grows when the dispersion increases from zero, and then gradually comes to a plateau. The only case, which differs from this trend is $g_k(\xi_k - x_k)$ for the uniform distribution as the consequence of the sharp edges of this function. Then a damped rippling takes place instead of the gradual transition to a plateau during an increase of the dispersion within the range of its high values. Nevertheless, all the studied dependencies of the rate of random transitions between the microstates on the dispersion of transition distance show a qualitative and sufficient quantitative similarity, including the tendency to unity at high dispersion values.

Thus, the shape of functions $g_k(\xi_k - x_k)$ does not exert a notable effect on the rate of damping of the spatial modes. The factors most influencing these modes are the dispersion of $(\xi_k - x_k)$ and the mode order m.

We have found that during the $D(\vec{x}, t)$ decay $\left(\text{i. e., during the } f(\vec{x}, t) \text{ approach to its equilibrium value, } \frac{1}{\Omega}\right)$ the initial profile of $D(\vec{x}, t)$ is invariable only in the case when random transitions occur with equal probability between all the microstates independently of their remoteness from one another. It takes place when the value of the dispersion $\frac{\sigma^2_{\xi_k}}{(L_k)^2}$ becomes close to 0.08 (see Fig. 2). For example, in the case of the uniform distribution $g_k(\xi_k - x_k)$ it means that the width of a "rectangle" of the random transition probability distribution equals L_k.

Otherwise, when such transitions are possible only within a limited range of distances between the microstates, the transient process has a more intricate profile. The higher the mode order m is, i. e., the more flexuous, spatially complicated profile the initial $D(\vec{x}, 0)$ has, the faster it decays. Therefore, $D(\vec{x}, t)$ (the deviation from the equilibrium value of $f(\vec{x}, t)$) not only diminishes in time but becomes more and more smooth. Finally, only a reminder of the first mode remains appreciable.

The expression for entropy, Eq. (50), obtained in this work, consists of two terms, the second of which shows how much the entropy of the nonequilibrium system is lower than its equilibrium value, when the value of $D(\vec{x}, t)$ is nonzero. Since this term is an integral, the flatness or, on the contrary, tortuosity of $D(\vec{x}, t)$ exerts not the biggest effect on the value of entropy in the nonequilibrium situation. Let us take into account that from the physical viewpoint the most real is the situation when random transitions are possible between the microscopic states, which are not very far from one another. From the above said, a conclusion can be made that it is the first mode of $D(\vec{x}, t)$ profile, which plays the main role in the expression of entropy.

A matter of separate interest is the rate of entropy change. In the case of an isolated system this quantity is, generally, the so-called rate of entropy production, $\frac{d_i S}{dt}$. It can be seen from the above said that this rate is specified by the quantity $D(\vec{x}, t)$ and by the rate of random transitions between the microstates, $\varphi(\vec{x}, \vec{\xi})$. Using formula transforms, we have obtained Eq. (52), in which one of the terms is described by Eq. (53). This result is in accord with the known formula [Kondepudi, Prigogine, 1998]

$$\frac{d_i S}{dt} = \sum_k X_k J_k,$$

where J_k are flows, and X_k are generalized forces, which give rise to these flows. In our case there are one flow and one generalized force. The latter equals the difference between the equilibrium value of entropy and two subtrahends. One of the latter is the entropy value, $S(t)$, existing at the present time. The second is $S_g(t)$, which is like the expression for entropy but also contains the quantity $g(\vec{\xi}, \vec{x})$ describing the rate of random transitions between the microstates. And the flow is proportional to the coefficient φ_0, which is present in the expression describing the rate of random transitions.

Increase of entropy in the case when the system initially is in a nonequilibrium state, and its maximality in the equilibrium state are the natural consequences of the presence of random transitions between the elements of the microscopic state set. Within this set there are no subsets isolated from one another, between which such transitions would be impossible. Therefore, an inevitable process is the system spread over the whole set of microscopic states and, as a result, the entropy convergence to its maximum.

Appendix 1. Transformation of divergence in the kinetic equation

The term with divergence in Eq. (1) can be transformed as follows:

$$\operatorname{div}(\vec{v}(\vec{x}) f(\vec{x}, t)) = \sum_{k=1}^{6N} \frac{\partial}{\partial x_k}(v_k(\vec{x}) f(\vec{x}, t)) = f(\vec{x}, t) \sum_{k=1}^{6N} \frac{\partial v_k(\vec{x})}{\partial x_k} + \sum_{k=1}^{6N} v_k(\vec{x}) \frac{\partial f(\vec{x}, t)}{\partial x_k}.$$

Further we use Hamilton equations Eqs. (3). In the numbering of k ($i = k$ when $k = 1 \div 3N$, and $i = k - 3N$ when $k = (3N + 1) \div 6N$) these equations take the form:

$$v_k(\vec{x}) = \frac{\partial H(\vec{x})}{\partial x_{k+3N}} \ (k = 1 \div 3N), \quad v_k(\vec{x}) = -\frac{\partial H(\vec{x})}{\partial x_{k-3N}} \ (k = (3N + 1) \div 6N).$$

From here:

$$\frac{\partial v_k(\vec{x})}{\partial x_k} = \frac{\partial^2 H(\vec{x})}{\partial x_k \, \partial x_{k+3N}} \ (k = 1 \div 3N), \quad \frac{\partial v_k(\vec{x})}{\partial x_k} = -\frac{\partial^2 H(\vec{x})}{\partial x_k \, \partial x_{k-3N}} \ (k = (3N + 1) \div 6N).$$

Further:

$$\sum_{k=1}^{6N} \frac{\partial v_k(\vec{x})}{\partial x_k} = \sum_{k=1}^{3N} \frac{\partial^2 H(\vec{x})}{\partial x_k \, \partial x_{k+3N}} - \sum_{k=3N+1}^{6N} \frac{\partial^2 H(\vec{x})}{\partial x_k \, \partial x_{k-3N}}.$$

Substitution of k by $m = k - 3N$ in the second term gives:

$$\sum_{k=1}^{6N} \frac{\partial v_k(\vec{x})}{\partial x_k} = \sum_{k=1}^{3N} \frac{\partial^2 H(\vec{x})}{\partial x_k \, \partial x_{k+3N}} - \sum_{m=1}^{3N} \frac{\partial^2 H(\vec{x})}{\partial x_{m+3N} \, \partial x_m} = 0,$$

from which we obtain that, when $\vec{x} = \begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix}$, the following equality takes place:

$$\operatorname{div}(\vec{v}(\vec{x}) f(\vec{x}, t)) = \sum_{k=1}^{6N} v_k(\vec{x}) \frac{\partial f(\vec{x}, t)}{\partial x_k}.$$

Appendix 2. Search for the entropy extremum

Applying conventional methods of variations calculus, we obtain that the condition of the extremum is:

$$\delta S^* = -\int\limits_{\mathrm{Surf_E}} \delta\{f(\vec{q}, \vec{p})[\ln f(\vec{q}, \vec{p}) - \lambda_1] - \lambda_2 (H(\vec{q}, \vec{p}) - E)\} \, d\vec{q} \, d\vec{p} = 0.$$

Variation of the integrand should equal zero, that gives the following expression:

$$\sum_{i=1}^{3N} \left\{ \frac{\partial f(\vec{q}, \vec{p})}{\partial q_i} [\ln f(\vec{q}, \vec{p}) - \lambda_1 + 1] \right\} \delta q_i + \sum_{i=1}^{3N} \left\{ \frac{\partial f(\vec{q}, \vec{p})}{\partial p_i} [\ln f(\vec{q}, \vec{p}) - \lambda_1 + 1] \right\} \delta p_i - \\ - \lambda_2 \left[\sum_{i=1}^{3N} \frac{\partial H(\vec{q}, \vec{p})}{\partial q_i} \delta q_i + \sum_{i=1}^{3N} \frac{\partial H(\vec{q}, \vec{p})}{\partial p_i} \delta p_i \right] = 0.$$

Since all δq_i and δp_i should belong to the surface $H(\vec{q}, \vec{p}) = E$, the expression in square brackets at the factor λ_2 equals zero according to that stated in Appendix 1. Therefore, all coefficients at all variations δq_i and δp_i should equal zero, from which the following two variants are possible: 1) all $\frac{\partial f(\vec{q}, \vec{p})}{\partial q_i} = 0$ and all $\frac{\partial f(\vec{q}, \vec{p})}{\partial p_i} = 0$; 2) $\ln f(\vec{q}, \vec{p}) - \lambda_1 + 1 = 0$. Solution of the first variant is $f(\vec{q}, \vec{p}) =$ $=$ const. Since λ_1 is constant, the second variant has the same solution: $f(\vec{q}, \vec{p}) =$ const.

Appendix 3. Values of entropy under deviations of the probability density within two arbitrary subregions of the system microstate set

Let us transform the expression (16):

$$S = \ln\Omega + \delta S = -\int\limits_{\mathrm{Surf}_{\mathrm{E}}^{1}} \left(\frac{1}{\Omega}+\delta f_1\right)\ln\left(\frac{1}{\Omega}+\delta f_1\right)d\vec{q}\,d\vec{p} - \int\limits_{\mathrm{Surf}_{\mathrm{E}}^{2}} \left(\frac{1}{\Omega}+\delta f_2\right)\ln\left(\frac{1}{\Omega}+\delta f_2\right)d\vec{q}\,d\vec{p} =$$

$$= -\left(\frac{1}{\Omega}+\delta f_1\right)\ln\left(\frac{1}{\Omega}+\delta f_1\right)\int\limits_{\mathrm{Surf}_{\mathrm{E}}^{1}} d\vec{q}\,d\vec{p} - \left(\frac{1}{\Omega}+\delta f_2\right)\ln\left(\frac{1}{\Omega}+\delta f_2\right)\int\limits_{\mathrm{Surf}_{\mathrm{E}}^{2}} d\vec{q}\,d\vec{p} =$$

$$= -\left(\frac{1}{\Omega}+\delta f_1\right)\ln\left(\frac{1}{\Omega}+\delta f_1\right)\Omega_1 - \left(\frac{1}{\Omega}+\delta f_2\right)\ln\left(\frac{1}{\Omega}+\delta f_2\right)\Omega_2.$$

Using the following interrelations:

$$\ln\left(\frac{1}{\Omega}+\delta f_{1,2}\right) = \ln\frac{1}{\Omega} + \ln\ln\left(1+\Omega\,\delta f_{1,2}\right),$$

$$\delta f_1 = \frac{1}{\Omega}\kappa_1, \quad \Omega_1 = \rho_1\Omega, \quad \Omega_2 = (1-\rho_1)\Omega, \quad \text{and} \quad \delta f_2 = -\frac{\rho_1}{1-\rho_1}\frac{1}{\Omega}\kappa_1,$$

we obtain

$$\ln\Omega + \delta S = -\Omega_1\frac{1}{\Omega}\ln\frac{1}{\Omega} - \Omega_2\frac{1}{\Omega}\ln\frac{1}{\Omega} - \Omega_1\,\delta f_1\ln\frac{1}{\Omega} - \Omega_2\,\delta f_2\ln\frac{1}{\Omega} -$$

$$- \frac{\Omega_1}{\Omega}(1+\Omega\,\delta f_1)\ln(1+\Omega\,\delta f_1) - \frac{\Omega_2}{\Omega}(1+\Omega\,\delta f_2)\ln(1+\Omega\,\delta f_2).$$

Further:

$$-\Omega_1\frac{1}{\Omega}\ln\frac{1}{\Omega} - \Omega_2\frac{1}{\Omega}\ln\frac{1}{\Omega} = -\ln\frac{1}{\Omega} = \ln\Omega;$$

and the following sum equals zero:

$$\Omega_1\,\delta f_1\ln\frac{1}{\Omega} - \Omega_2\,\delta f_2\ln\frac{1}{\Omega} = 0$$

as a result of the normalizing condition imposed on δf_1 and δf_2. Finally, we obtain:

$$\delta S = -\rho_1(1+\kappa_1)\ln(1+\kappa_1) - (1-\rho_1)\left(1+\frac{\rho_1}{1-\rho_1}\kappa_1\right)\ln\left(1+\frac{\rho_1}{1-\rho_1}\kappa_1\right).$$

Appendix 4. Calculation of the integral in Eq. (38)

$$\int\limits_{x_k-L_k/2}^{x_k+L_k/2} g_k(\xi_k,\,x_k)D_{km}(x_k)\,d\xi_k =$$

$$= A_{km}\int\limits_{x_k-L_k/2}^{x_k+L_k/2} g_k(\xi_k,\,x_k)\cos\left(2\pi m\frac{x_k}{L_k}\right)d\xi_k + B_{km}\int\limits_{x_k-L_k/2}^{x_k+L_k/2} g_k(\xi_k,\,x_k)\sin\left(2\pi m\frac{x_k}{L_k}\right)d\xi_k. \quad (38)$$

In the present work we consider functions g_k symmetrically dependent on their arguments:

$$g_k(\xi_k,\, x_k) = g_k(\xi_k - x_k) = g_k(x_k - \xi_k).$$

Let us represent the argument of cosine and sine as follows:

$$2\pi m\frac{\xi_k}{L_k} = 2\pi m\frac{\xi_k - x_k}{L_k} + 2\pi m\frac{x_k}{L_k}.$$

We use here the known formulae:

$$\cos(\alpha+\beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta) \quad \text{and} \quad \sin(\alpha+\beta) = \sin(\alpha)\cos(\beta) + \cos(\alpha)\sin(\beta)$$

at $\alpha = 2\pi m\frac{\xi_k - x_k}{L_k}$ and $\beta = 2\pi m\frac{x_k}{L_k}$. Then

$$\int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k - x_k) D_{km}(\xi_k)\, d\xi_k =$$

$$= \left[A_{km}\cos\left(2\pi m\frac{x_k}{L_k}\right) + B_{km}\sin\left(2\pi m\frac{x_k}{L_k}\right)\right] \cdot \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k - x_k)\cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right) d\xi_k +$$

$$+ \left[B_{km}\cos\left(2\pi m\frac{x_k}{L_k}\right) - A_{km}\sin\left(2\pi m\frac{x_k}{L_k}\right)\right] \cdot \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k - x_k)\sin\left(2\pi m\frac{\xi_k - x_k}{L_k}\right) d\xi_k.$$

The second integral in this expression is taken from an antisymmetric function within symmetric limits. Therefore, it equals zero. Taking Eq. (37) into account, we obtain:

$$\int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k - x_k) D_{km}(\xi_k)\, d\xi_k = D_{km}(x_k) \cdot \int\limits_{x_k - L_k/2}^{x_k + L_k/2} g_k(\xi_k - x_k)\cos\left(2\pi m\frac{\xi_k - x_k}{L_k}\right) d\xi_k. \tag{55}$$

Appendix 5. Transformation of Eq. (51)

The rate of entropy change has the form:

$$\frac{dS}{dt} = \varphi_0\Omega \int\limits_{\mathrm{Surf_E}} D(\vec{x},\, t)\ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x} - \varphi_0\Omega \int\limits_{\mathrm{Surf_E}} \left[\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x}) D(\vec{\xi},\, t)\, d\vec{\xi}\right] \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x}. \tag{51}$$

Transform of the second term in the right-hand side of (51):

$$-\varphi_0\Omega \int\limits_{\mathrm{Surf_E}} \left[\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x}) D(\vec{\xi},\, t)\, d\vec{\xi}\right] \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x} =$$

$$= -\varphi_0 \int\limits_{\mathrm{Surf_E}} \left[\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x})(1 + \Omega D(\vec{\xi},\, t))\, d\vec{\xi}\right] \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x} +$$

$$+ \varphi_0 \int\limits_{\mathrm{Surf_E}} \left[\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x})\, d\vec{\xi}\right] \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x}.$$

Since $\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x})\, d\vec{\xi} = 1$, this expression equals

$$-\varphi_0 \int\limits_{\mathrm{Surf_E}} \left[\int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x})(1 + \Omega D(\vec{\xi},\, t))\, d\vec{\xi} \right] \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x} + \varphi_0 \int\limits_{\mathrm{Surf_E}} \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x}.$$

Substituting this expression into Eq. (51), we obtain:

$$\frac{dS}{dt} = \varphi_0 \int\limits_{\mathrm{Surf_E}} (1 + \Omega D(\vec{x},\, t)) \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{x} - \\ - \varphi_0 \int\limits_{\mathrm{Surf_E}} \int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x})(1 + \Omega D(\vec{\xi},\, t)) \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{\xi}\, d\vec{x}. \quad (56)$$

Introduce the following denotation:

$$S_g = \frac{1}{\Omega} \int\limits_{\mathrm{Surf_E}} \int\limits_{\mathrm{Surf_E}} g(\vec{\xi},\, \vec{x})(1 + \Omega D(\vec{\xi},\, t)) \ln(1 + \Omega D(\vec{x},\, t))\, d\vec{\xi}\, d\vec{x}. \quad (57)$$

Further we use the expression for entropy:

$$S(t) = \ln \Omega - \frac{1}{\Omega} \int\limits_{\mathrm{Surf_E}} (1 + \Omega D(\vec{x},\, t))[\ln(1 + \Omega D(\vec{x},\, t))]\, d\vec{x}, \quad (50)$$

from which we find:

$$\int\limits_{\mathrm{Surf_E}} (1 + \Omega D(\vec{x},\, t))[\ln(1 + \Omega D(\vec{x},\, t))]\, d\vec{x} = \Omega(\ln \Omega - S(t)). \quad (58)$$

Substituting Eqs. (58) and (57) into Eq. (56), we obtain a general expression for the rate of entropy change:

$$\frac{dS}{dt} = \varphi_0 \Omega [\ln \Omega - S(t) - S_g(t)].$$

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