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# Stationary solutions of Liouville equations for non-Hamiltonian systems

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**Abstract**

We consider the class of non-Hamiltonian and dissipative statistical systems with distributions that are determined by the Hamiltonian. The distributions are derived analytically as stationary solutions of the Liouville equation for non-Hamiltonian systems. The class of non-Hamiltonian systems can be described by a non-holonomic (non-integrable) constraint: the velocity of the elementary phase volume change is directly proportional to the power of non-potential forces. The coefficient of this proportionality is determined by Hamiltonian. The constant temperature systems, canonical–dissipative systems, and Fermi–Bose classical systems are the special cases of this class of non-Hamiltonian systems.


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## 1. Introduction

The canonical distribution for the Hamiltonian systems was defined by Gibbs in the book “Elementary principles in statistical mechanics” [1], published in 1902. In general, classical systems are not Hamiltonian systems and the forces are the sum of

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potential and non-potential forces. Non-Hamiltonian and dissipative systems can have the same distributions as Hamiltonian systems. The canonical distributions for the non-Hamiltonian and dissipative systems were considered in [2–5,7,8,6,9–11].

The aim of this work is the extension of the statistical mechanics of conservative Hamiltonian systems to a wide class of non-Hamiltonian and dissipative systems.

Let us point out non-Hamiltonian systems with distribution functions that are defined by the Hamiltonian.

(1) In the papers [2–6,9], the constant temperature systems with minimal Gaussian constraint are considered. These systems are the non-Hamiltonian systems that are described by the non-potential forces in the form $\mathbf{F}_i^{(n)} = -\gamma \mathbf{p}_i$ and the Gaussian non-holonomic constraint. Note that this constraint can be represented as an addition term to the non-potential force.
(2) In the papers [12,13], the canonical–dissipative systems are considered. These systems are the non-Hamiltonian systems that are described by the non-potential forces $\mathbf{F}_i^{(n)} = -\partial G(H)/\partial \mathbf{p}_i$, where $G(H)$ is a function of Hamiltonian $H$. Note that the distribution functions are derived as solutions the Fokker–Planck equation. It is known that Fokker–Planck equation can be derived from the Liouville equation [14].
(3) In the paper [15], the systems with non-holonomic constraint and non-potential forces $\mathbf{F}_i^{(n)} = 0$ are considered. The equations of motion for this system are incorrect [16]. The correct form of the equations is derived in [15] by the limit $\tau \to 0$. This procedure removes the incorrect term of the equations.
(4) In the paper [11], the canonical distribution is considered as a stationary solution of the Liouville equation for a wide class of non-Hamiltonian system. This class is defined by a very simple condition for the non-potential forces: the power of the non-potential forces must be directly proportional to the velocity of the Gibbs phase (elementary phase volume) change. This condition defines the general constant temperature systems. Note that the condition is a non-holonomic constraint. This constraint leads to the canonical distribution as a stationary solution of the Liouville equations. For the linear friction, we derived the constant temperature systems. The general form of the non-potential forces is not derived in [11].
(5) In the paper [17], the quantum non-Hamiltonian systems with pure stationary states are considered. The correspondent classical systems are not discussed.
(6) In the paper [19], the non-Gaussian distributions are suggested for the non-Hamiltonian systems in the fractional phase space. Note that non-dissipative systems with the usual phase space are dissipative systems in the fractional phase space [19].

Khintchin [20] revealed the deep relation between the Gaussian central limit theorem and canonical Gibbs distribution. However, the Gaussian central limit theorem is non-unique. Levy and Khintchin have generalized the Gaussian central limit theorem to the case of summation of independent, identically distributed random variables which are described by long tailed distributions. In this case, non-Gaussian distributions replace the Gaussian in the generalized limit theorems. It is interesting to find statistical mechanics and thermodynamics that is based on non-Gaussian and non-canonical distributions [21–24].

The aim of this paper is the description of non-Hamiltonian and dissipative systems with (canonical and non-canonical) distributions that are defined by Hamiltonian. This class can be described by the non-holonomic (non-integrable) constraint: the velocity of the elementary phase volume change must be directly proportional to the power of non-potential forces. The coefficient of this proportionality is determined by the Hamiltonian. These distributions can be derived analytically as solutions of the Liouville equation for non-Hamiltonian systems. The special constraint allows us to derive solutions for the system, even in far-from equilibrium states. This class of the non-Hamiltonian systems is characterized by the distribution functions that are determined by the Hamiltonian. The constant temperature systems [2–6,9], the canonical–dissipative systems [12,13], and the Fermi–Bose classical systems [13] are the special cases of suggested class of non-Hamiltonian systems.

In Section 2, the definitions of the non-Hamiltonian and dissipative systems, mathematical background and notations are considered. In Section 3, we consider the condition for the non-potential forces. We formulate the proposition that allows us to answer the following question: Is this system a canonical non-Hamiltonian system? We derive the solution of the $N$-particle Liouville equation for the non-Hamiltonian systems with non-holonomic constraint. In Section 4, we consider the non-holonomic constraint for non-Hamiltonian systems. We formulate the proposition which allows us to derive the canonical non-Hamiltonian systems from the equations of non-Hamiltonian system motion. The non-Hamiltonian systems with the simple Hamiltonian and the simple non-potential forces are considered. In Section 5, we derive the class of non-Hamiltonian systems with canonical Gibbs distribution as a solution of the Liouville equation. In Section 6, we consider the non-Gaussian distributions as solutions of the Liouville equations for the non-Hamiltonian systems. In Section 7, we derive the analog of thermodynamics laws for the non-Hamiltonian systems with the distributions that are defined by Hamiltonian. Finally, a short conclusion is given in Section 8.

## 2. Definitions of non-Hamiltonian, dissipative, and canonical non-Hamiltonian systems

Let us consider the definitions of non-Hamiltonian and dissipative classical systems [25], which are used for the formulation of our results.

Usually a classical system is called a Hamiltonian system if the equations of motion are determined by Hamiltonian. The more consistent definition of the non-Hamiltonian system is connected with Helmholtz condition for the equation of motion.

**Definition 1.** A classical system which is defined by the equations

$$\frac{dq_i}{dt} = G_i, \quad \frac{dp_i}{dt} = F_i, \tag{1}$$

where $i = 1, \ldots, N$, is called Hamiltonian system if the right-hand sides of Eq. (1) satisfy the Helmholtz conditions for the phase space

$$\frac{\partial G_i}{\partial p_j} - \frac{\partial G_j}{\partial p_i} = 0, \quad \frac{\partial F_i}{\partial p_j} + \frac{\partial G_j}{\partial q_i} = 0, \quad \frac{\partial F_i}{\partial q_j} - \frac{\partial F_j}{\partial q_i} = 0. \tag{2}$$

Here $G_i = G_i(q,p)$, $F_i = F_i(q,p,a,t)$, where $a$ is a set of external parameters.

If the Helmholtz conditions are satisfied, then the equations of motion for the system (1) can be represented as canonical equations

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{\partial H}{\partial p_i}, \quad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i}, \tag{3}$$

which are completely characterized by the Hamiltonian $H = H(q,p,a)$. In this case, the forces, which act on the particles are potential forces.

If the functions $G_i$ for the non-Hamiltonian system (1) are determined by the Hamiltonian

$$G_i = \frac{\partial H}{\partial p_i} \tag{4}$$

and the Hamiltonian is a smooth function on the momentum space, then the first condition (2) is satisfied

$$\frac{\partial^2 H}{\partial p_i \partial p_j} - \frac{\partial^2 H}{\partial p_j \partial p_i} = 0.$$

In this case, the second condition (2) has the form

$$\frac{\partial F_i}{\partial p_j} + \frac{\partial^2 H}{\partial q_i \partial p_j} = 0. \tag{5}$$

In general, the second term does not vanish. For example, in the non-linear one-dimensional sigma-model [27] the second term of the left-hand side of Eq. (5) is defined by the metric.

**Definition 2.** A mechanical system is called non-Hamiltonian if at least one of conditions (2) is not satisfied.

Let us consider the time evolution of the classical state which is defined by the distribution function $\rho_N(q,p,a,t)$. The $N$-particle distribution function in the Hamilton picture (for the Euler variables) is normalized by the condition

$$\int \rho_N(q,p,a,t)\mathrm{d}^N q\, \mathrm{d}^N p = 1. \tag{6}$$

The evolution equation of the distribution function $\rho_N(q,p,a,t)$ is Liouville equation in the Hamilton picture

$$\frac{\mathrm{d}\rho_N(q,p,a,t)}{\mathrm{d}t} = -\Omega(q,p,a,t)\,\rho_N(q,p,a,t). \tag{7}$$

This equation describes the change of the distribution function $\rho_N$ along the trajectory in the $6N$-dimensional phase space. Here, $\Omega$ is defined by

$$\Omega(q,p,a,t) = \frac{\partial F_i}{\partial p_i} + \frac{\partial G_i}{\partial q_i}. \tag{8}$$

Here and later we mean the sum on the repeated index $i$ from 1 to $N$. Derivative $\mathrm{d}/\mathrm{d}t$ is a total time derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + G_i \frac{\partial}{\partial q_i} + F_i \frac{\partial}{\partial p_i}. \tag{9}$$

If the vector function $G_i$ is defined by Eq. (4), then

$$\Omega(q,p,a,t) = \frac{\partial F_i}{\partial p_i} + \frac{\partial^2 H}{\partial q_i \partial p_i}.$$

In general, the second term does not vanish, for example, in the non-linear one-dimensional sigma-model [27].

In the Liouville picture (for the Lagrange variables) the function $\Omega$ defines the velocity of the phase volume change [26]

$$\frac{\mathrm{d}V_{\mathrm{ph}}(a,t)}{\mathrm{d}t} = \int \Omega(q,p,a,t)\mathrm{d}^N q\, \mathrm{d}^N p.$$

**Definition 3.** If $\Omega \leqslant 0$ for all phase space points $(q,p)$ and $\Omega < 0$ for some points of phase space, then the system is called a dissipative system.

We can define dissipative system using a phase density of entropy

$$S(q,p,a,t) = -k \ln \rho_N(q,p,a,t).$$

This function usually called the Gibbs phase. Eq. (7) leads to the equation for the entropy density (Gibbs phase)

$$\frac{\mathrm{d}S(q,p,a,t)}{\mathrm{d}t} = k\Omega(q,p,a,t). \tag{10}$$

It is easy to see that the function $\Omega$ is proportional to the velocity of the phase entropy density change. Therefore, the dissipative systems can be defined by the following equivalent definition.

**Definition 4.** A system is called a generalized dissipative system if the velocity of the entropy density change does not equal to zero.

Let us define the special class of the non-Hamiltonian systems with distribution functions that are completely characterized by the Hamiltonian. These distributions can be derived analytically as stationary solutions of the Liouville equation for the non-Hamiltonian system.

**Definition 5.** A non-Hamiltonian system will be called a canonical non-Hamiltonian system if the distribution function is determined by the Hamiltonian, i.e., $\rho_N(q,p,a)$ can be written in the form

$$\rho_N(q,p,a) = \rho_N(H(q,p,a),a), \tag{11}$$

where $a$ is a set of external parameters.

Examples of the canonical non-Hamiltonian systems:

(1) The constant temperature systems [2–6,9] that have the canonical distribution. In general, these systems can be defined by the non-holonomic constraint, which is suggested in [11].
(2) The Fermi–Bose canonical–dissipative systems [13] which are defined by the distribution functions in the form

$$\rho_N(H(q,p,a)) = \frac{1}{\exp(\beta(H(q,p,a)-\mu)+s)}. \tag{12}$$

(3) The classical system with the Breit–Wigner distribution function is defined by

$$\rho_N(H) = \frac{\lambda}{(H-E)^2+(\Gamma/2)^2}. \tag{13}$$

## 3. Distribution as a solution of the Liouville equation

### 3.1. Formulation of the results

Let us formulate the proposition that allows us to answer the following question: Is this system a canonical non-Hamiltonian system?

Let us consider the $N$-particle non-Hamiltonian systems which are defined by the equations

$$\frac{d\mathbf{r}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial H}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(n)}. \tag{14}$$

The power of non-potential forces is defined by

$$\mathscr{P}(\mathbf{r},\mathbf{p},a) = \mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}. \tag{15}$$

If the power of the non-potential forces is equal to zero ($\mathscr{P}=0$) and $\partial H/\partial t = 0$, then classical system is called a conservative system. The velocity of an elementary phase volume change $\Omega$ is defined by the equation

$$\Omega(\mathbf{r},\mathbf{p},a) = \frac{\partial \mathbf{F}_i}{\partial \mathbf{p}_i} + \frac{\partial^2 H}{\partial \mathbf{r}_i \partial \mathbf{p}_i} = \frac{\partial \mathbf{F}_i^{(n)}}{\partial \mathbf{p}_i}. \tag{16}$$

We use the following notations for the scalar product:

$$\frac{\partial \mathbf{A}_i}{\partial \mathbf{a}_i} = \sum_{i=1}^{N} \left( \frac{\partial A_{xi}}{\partial a_{xi}} + \frac{\partial A_{yi}}{\partial a_{yi}} + \frac{\partial A_{zi}}{\partial a_{zi}} \right).$$

The aim of this section is to prove the following result.

**Proposition 1.** *If the non-potential forces* $\mathbf{F}_i^{(n)}$ *of the non-Hamiltonian system* (14) *satisfy the constraint condition*

$$g(H)\mathbf{F}_i^{(n)}\frac{\partial H}{\partial \mathbf{p}_i} - \frac{\partial \mathbf{F}_i^{(n)}}{\partial \mathbf{p}_i} = 0, \tag{17}$$

*then this system is a canonical non-Hamiltonian system with the distribution function*

$$\rho_N(\mathbf{r}, \mathbf{p}, a) = Z(a)\exp(-L(H(\mathbf{r}, \mathbf{p}, a))), \tag{18}$$

*where the function* $L(H)$ *is defined by the equation*

$$g(H) = \frac{\partial L(H)}{\partial H}. \tag{19}$$

*The condition* (17) *can be formulated in other words*: *If velocity of the elementary phase volume change* $\Omega$ *is directly proportional to the power* $\mathcal{P}$ *of non-potential forces* $\mathbf{F}_i^{(n)}$ *of the non-Hamiltonian system* (14) *and coefficient of this proportionality is a function* $g(H)$ *of Hamiltonian* $H$, *i.e.*,

$$\Omega(\mathbf{r}, \mathbf{p}, t) - g(H)\mathcal{P}(\mathbf{r}, \mathbf{p}, t) = 0, \tag{20}$$

*then this system is a canonical non-Hamiltonian system.*

Note that any non-Hamiltonian system with the non-holonomic constraint (20) or (17) is a canonical non-Hamiltonian system.

**Example.** Let us consider $g(H) = 3N\beta(a)$, where $\beta(a) = 1/kT(a)$. This case is considered in [11]. If we consider the $N$-particle system with the Hamiltonian

$$H(\mathbf{r}, \mathbf{p}, a) = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + U(\mathbf{r}, a) \tag{21}$$

and a linear friction, which is defined by the non-potential forces

$$\mathbf{F}_i^{(n)} = -\gamma \mathbf{p}_i, \tag{22}$$

then the non-holonomic constraint (17) has the form

$$\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{m} = kT(a), \tag{23}$$

i.e., the kinetic energy of the system must be a constant. The constraint (23) is a non-holonomic minimal Gaussian constraint [11,9].

If the function $g(H)$ is defined by $g(H) = 3N\beta(a)$, then the non-Hamiltonian system can have the canonical Gibbs distribution [11]. The classical systems that are defined by Eqs. (21)–(23) are canonical non-Hamiltonian systems.

### 3.2. Proof of the result

Solving the Liouville equation with the non-holonomic constraint (17), we can obtain the (canonical and non-canonical) distributions that are defined by the Hamiltonian.

Let us consider the Liouville equation for the $N$-particle distribution function $\rho_N = \rho_N(\mathbf{r}, \mathbf{p}, a, t)$. This distribution function $\rho_N$ express a probability that a phase space point $(\mathbf{r}, \mathbf{p})$ will appear. The Liouville equation for this non-Hamiltonian system

$$\frac{\partial \rho_N}{\partial t} + \frac{\partial}{\partial \mathbf{r}_i}(\mathbf{G}_i \rho_N) + \frac{\partial}{\partial \mathbf{p}_i}(\mathbf{F}_i \rho_N) = 0 \tag{24}$$

expresses the conservation of probability in the phase space. Here, we use

$$\mathbf{G}_i = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \mathbf{F}_i = -\frac{\partial H}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(n)}.$$

We define a total time derivative along the phase space trajectory by

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{G}_i \frac{\partial}{\partial \mathbf{r}_i} + \mathbf{F}_i \frac{\partial}{\partial \mathbf{p}_i}. \tag{25}$$

Therefore Eq. (24) can be written in the form (7)

$$\frac{\mathrm{d}\rho_N}{\mathrm{d}t} = -\Omega \rho_N, \tag{26}$$

where the omega function is defined by Eq. (16). In classical mechanics of Hamiltonian systems the right-hand side of the Liouville equation (26) is zero, and the distribution function does not change in time. For the non-Hamiltonian systems (14), the omega function (16) does not vanish. For this system, the omega function is defined by Eq. (16). For the canonical non-Hamiltonian systems, this function is defined by the constraint (17) in the form

$$\Omega = g(H) \mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}.$$

In this case, the Liouville equation has the form

$$\frac{\mathrm{d}\rho_N}{\mathrm{d}t} = -g(H) \mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i} \rho_N. \tag{27}$$

Let us consider the total time derivative of the Hamiltonian. Using equations of motion (14), we have

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t} + \frac{\partial H}{\partial \mathbf{p}_i}\frac{\partial H}{\partial \mathbf{r}_i} + \left(-\frac{\partial H}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(n)}\right)\frac{\partial H}{\partial \mathbf{p}_i} = \frac{\partial H}{\partial t} + \mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}.$$

If $\partial H/\partial t = 0$, then the power $\mathscr{P}$ of non-potential forces is equal to the total time derivative of the Hamiltonian

$$\mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i} = \frac{\mathrm{d}H}{\mathrm{d}t}.$$

Eq. (27) can be written in the form

$$\frac{d\rho_N}{dt} = -g(H)\frac{dH}{dt}\rho_N. \tag{28}$$

Let us consider the following form of this equation:

$$\frac{d\ln\rho_N}{dt} = -g(H)\frac{dH}{dt}. \tag{29}$$

If $g(H)$ is an integrable function, then this function can be represented as a derivative

$$g(H) = \frac{\partial L(H)}{\partial H}. \tag{30}$$

In this case, we can write Eq. (29) in the form

$$\frac{d\ln\rho_N}{dt} = -\frac{dL(H)}{dt}. \tag{31}$$

As a result, we have the following solution of the Liouville equation:

$$\rho_N(\mathbf{r}, \mathbf{p}, a) = Z(a)\exp(-L(H(\mathbf{r}, \mathbf{p}, a))). \tag{32}$$

The function $Z(a)$ is defined by the normalization condition. It is easy to see that the distribution function of the non-Hamiltonian system is determined by the Hamiltonian. Therefore, this system is a canonical non-Hamiltonian system.

Note that $N$ is an arbitrary natural number since we do not use the condition $N \gg 1$ or $N \to \infty$.

## 4. Non-holonomic constraint for non-Hamiltonian systems

### 4.1. Formulation of the result

Let us formulate the proposition which allows us to derive the canonical non-Hamiltonian systems from any equations of motion of non-Hamiltonian systems.

The aim of this section is to prove the following result.

**Proposition 2.** *For any non-Hamiltonian system which is defined by the equation*

$$\frac{d\mathbf{r}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i, \tag{33}$$

*where $\mathbf{F}_i$ is the sum of potential and non-potential forces*

$$\mathbf{F}_i = -\frac{\partial H}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(n)}, \tag{34}$$

*there exists a canonical non-Hamiltonian system that is defined by the equations*

$$\frac{d\mathbf{r}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i^{\mathrm{new}}, \tag{35}$$

*where the non-potential forces* $\mathbf{F}_i^{\text{new}}$ *are defined by*

$$\mathbf{F}_i^{\text{new}} = \frac{\mathbf{A}_k\mathbf{A}_k\delta_{ij} - \mathbf{A}_i\mathbf{A}_j}{\mathbf{A}_k\mathbf{A}_k}\mathbf{F}_j - \frac{\mathbf{A}_i\mathbf{B}_j}{\mathbf{A}_k\mathbf{A}_k}\frac{\partial H}{\partial \mathbf{p}_j}. \tag{36}$$

*The vectors* $\mathbf{A}_i$ *and* $\mathbf{B}_i$ *are defined by the equations*

$$\mathbf{A}_i = \frac{\partial g(H)}{\partial H}\frac{\partial H}{\partial \mathbf{p}_i}\frac{\partial H}{\partial \mathbf{p}_j}\mathbf{F}_j^{(n)} + g(H)\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_i}\frac{\partial H}{\partial \mathbf{p}_j} + g(H)\mathbf{F}_j^{(n)}\frac{\partial^2 H}{\partial \mathbf{p}_i \partial \mathbf{p}_j} - \frac{\partial^2 \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_i \partial \mathbf{p}_j} \tag{37}$$

*and*

$$\mathbf{B}_i = \frac{\partial g(H)}{\partial H}\frac{\partial H}{\partial \mathbf{r}_i}\frac{\partial H}{\partial \mathbf{p}_j}\mathbf{F}_j^{(n)} + g(H)\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{r}_i}\frac{\partial H}{\partial \mathbf{p}_j} + g(H)\mathbf{F}_j^{(n)}\frac{\partial^2 H}{\partial \mathbf{r}_i \partial \mathbf{p}_j} - \frac{\partial^2 \mathbf{F}_j^{(n)}}{\partial \mathbf{r}_i \partial \mathbf{p}_j}. \tag{38}$$

Note that the forces that are defined by Eqs. (36)–(38) satisfy the non-holonomic constraint (20), i.e.,

$$g(H)\mathbf{F}_j^{\text{new}}\frac{\partial H}{\partial \mathbf{p}_j} - \frac{\partial \mathbf{F}_j^{\text{new}}}{\partial \mathbf{p}_j} - \frac{\partial^2 H}{\partial \mathbf{r}_j \partial \mathbf{p}_j} = 0. \tag{39}$$

### 4.2. Proof. Part I

In this section, we prove Eq. (36).

Let us consider the $N$-particle classical system in the Hamilton picture. Denote the position of the $i$th particle by $\mathbf{r}_i$ and its momentum by $\mathbf{p}_i$.

Suppose that the system is subjected to a non-holonomic (non-integrable) constraint in the form

$$f(\mathbf{r}, \mathbf{p}) = 0. \tag{40}$$

Differentiation of Eq. (40) with respect to time gives a relation

$$\mathbf{A}_i(\mathbf{r}, \mathbf{p})\frac{d\mathbf{p_i}}{dt} + \mathbf{B}_i(\mathbf{r}, \mathbf{p})\frac{d\mathbf{r_i}}{dt} = 0, \tag{41}$$

where

$$\mathbf{A}_i(\mathbf{r}, \mathbf{p}) = \frac{\partial f}{\partial \mathbf{p}_i}, \quad \mathbf{B}_i(\mathbf{r}, \mathbf{p}) = \frac{\partial f}{\partial \mathbf{r}_i}. \tag{42}$$

An unconstrained motion of the $i$th particle, where $i = 1, \ldots, N$, is described by the equations

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{G}_i, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i, \tag{43}$$

where $\mathbf{F}_i$ is a resulting force, which acts on the $i$th particle.

The unconstrained motion gives a trajectory which leaves the constraint hypersurface (40). The constraint forces $\mathbf{R}_i$ must be added to the equation of motion to prevent the deviation from the constraint hypersurface

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{G}_i, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i + \mathbf{R}_i. \tag{44}$$

The constraint force $\mathbf{R}_i$ for the non-holonomic constraint is proportional to the $\mathbf{A}_i$ [16]

$$\mathbf{R}_i = \lambda \mathbf{A}_i, \tag{45}$$

where the coefficient $\lambda$ of the constraint force term is an undetermined Lagrangian multiplier. For the non-holonomic constraint (40), the equations of motion (43) are modified as

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{G}_i, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i + \lambda \mathbf{A}_i. \tag{46}$$

The Lagrangian coefficient $\lambda$ is determined by Eq. (41). Substituting Eq. (44) into Eq. (41), we get

$$\mathbf{A}_i(\mathbf{F}_i + \lambda \mathbf{A}_i) + \mathbf{B}_i \mathbf{G}_i = 0. \tag{47}$$

Therefore, the Lagrange multiplier $\lambda$ is equal to

$$\lambda = -\frac{\mathbf{A}_i \mathbf{F}_i + \mathbf{B}_i \mathbf{G}_i}{\mathbf{A}_k \mathbf{A}_k}. \tag{48}$$

As a result, we obtain the following equations:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{G}_i, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i - \mathbf{A}_i \frac{\mathbf{A}_j \mathbf{F}_j + \mathbf{B}_j \mathbf{G}_j}{\mathbf{A}_k \mathbf{A}_k}. \tag{49}$$

These equations we can rewrite in the form (43)

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{G}_i, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i^{\text{new}} \tag{50}$$

with the new forces

$$\mathbf{F}_i^{\text{new}} = \frac{\mathbf{A}_k \mathbf{A}_k \delta_{ij} - \mathbf{A}_i \mathbf{A}_j}{\mathbf{A}_k \mathbf{A}_k} \mathbf{F}_j - \frac{\mathbf{A}_i \mathbf{B}_j}{\mathbf{A}_k \mathbf{A}_k} \mathbf{G}_j. \tag{51}$$

In general, the forces $\mathbf{F}_i^{\text{new}}$ are non-potentials forces (see examples in [11]).

Eq. (49) are equations of the *holonomic* non-Hamiltonian system. For any trajectory of the system in the phase space, we have $f = \text{const}$. If initial values $\mathbf{r}_k(0)$ and $\mathbf{p}_k(0)$ satisfy the constraint condition $f(\mathbf{r}(0), \mathbf{p}(0)) = 0$, then solution of Eqs. (49) and (51) is a motion of the non-holonomic system.

### 4.3. Proof. Part II

In this section, we prove Eqs. (37) and (38).

Let us consider the non-Hamiltonian system (43) with

$$\mathbf{G}_i = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \mathbf{F}_i = -\frac{\partial H}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(n)} \tag{52}$$

and the special form of the non-holonomic constraint (40). Let us assume the following constraint: the velocity of the elementary phase volume change $\Omega(\mathbf{r},\mathbf{p},a)$ is directly proportional to the power $\mathscr{P}(\mathbf{r}, \mathbf{p}, a)$ of the non-potential forces, i.e.,

$$\Omega(\mathbf{r},\mathbf{p},a) = g(H)\mathscr{P}(\mathbf{r},\mathbf{p},a), \tag{53}$$

where $g(H)$ depends on the Hamiltonian $H$. Therefore, the system is subjected to a non-holonomic (non-integrable) constraint (40) in the form

$$f(\mathbf{r},\mathbf{p},a) = g(H)\mathscr{P}(\mathbf{r},\mathbf{p},a) - \Omega(\mathbf{r},\mathbf{p},a) = 0. \tag{54}$$

This constraint is a generalization of the condition which is suggested in [11]. The power $\mathscr{P}$ of the non-potential forces $\mathbf{F}_i^{(n)}$ is defined by Eq. (15). The function $\Omega$ is defined by Eq. (16).

Eq. (54) for the non-potential forces has the form

$$g(H)\mathbf{F}_j^{(n)}\frac{\partial H}{\partial \mathbf{p}_j} - \frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_j} = 0.$$

Let us find the functions $\mathbf{A}_i$ and $\mathbf{B}_i$ for this constraint. Differentiation of the function $f(\mathbf{r},\mathbf{p},a)$ with respect to $\mathbf{p}_i$ gives

$$\mathbf{A}_i = \frac{\partial f}{\partial \mathbf{p}_i} = \frac{\partial}{\partial \mathbf{p}_i}\left(g(H)\mathbf{F}_j^{(n)}\frac{\partial H}{\partial \mathbf{p}_j}\right) - \frac{\partial}{\partial \mathbf{p}_i}\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_j}.$$

Therefore we obviously have (37). Differentiation of the function $f(\mathbf{r},\mathbf{p},a)$ with respect to $\mathbf{r}_i$ gives

$$\mathbf{B}_i = \frac{\partial f}{\partial \mathbf{r}_i} = \frac{\partial}{\partial \mathbf{r}_i}\left(g(H)\mathbf{F}_j^{(n)}\frac{\partial H}{\partial \mathbf{p}_j}\right) - \frac{\partial}{\partial \mathbf{r}_i}\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_j}.$$

Therefore, we have (38).

### 4.4. Minimal constraint models

To realize simulation of the classical systems with canonical and non-canonical distributions, we must have the simple constraints. Let us consider the minimal constraint models which are defined by the simplest form of the Hamiltonian and the non-potential forces

$$H(\mathbf{r},\mathbf{p},a) = \frac{\mathbf{p}^2}{2m} + U(\mathbf{r},a), \quad \mathbf{F}_i^{(n)} = -\gamma \mathbf{p}_i. \tag{55}$$

where $\mathbf{p}^2 = \sum_{i=1}^N \mathbf{p}_i^2$. For these models, the non-holonomic constraint is defined by the equation

$$f = g(H)\frac{\mathbf{p}^2}{m} - 3N = 0, \tag{56}$$

where $N$ is the number of particles. The phase space gradients (37) and (38) of the constraint can be represented in the form

$$\mathbf{A}_i = \left(\frac{\partial g(H)}{\partial H}\frac{\mathbf{p}^2}{2m} + g(H)\right)\frac{2\mathbf{p}_i}{m}, \quad \mathbf{B}_i = \frac{\partial g(H)}{\partial H}\frac{\partial H}{\partial \mathbf{r}_i}.$$

The non-potential forces of the minimal constraint models have the form

$$\mathbf{F}_i = -\frac{\mathbf{p}^2\delta_{ij} - \mathbf{p}_i\mathbf{p}_j}{\mathbf{p}^2}\frac{\partial U}{\partial \mathbf{r}_j} + \frac{\mathbf{p}_i\mathbf{p}_j}{2\mathbf{p}^2((\mathbf{p}^2/2m)(\partial g(H)/\partial H) + g(H))}\frac{\partial g(H)}{\partial H}\frac{\partial U}{\partial \mathbf{r}_j}.$$

It is easy to see that all minimal constraint models have the potential forces.

For the minimal Gaussian constraint model

$$\frac{\partial g(H)}{\partial H} = 0,$$

we have the non-potential forces in the form

$$\mathbf{F}_i = -\frac{\partial U}{\partial \mathbf{r}_j}\frac{\mathbf{p}^2\delta_{ij} - \mathbf{p}_i\mathbf{p}_j}{\mathbf{p}^2}.$$

This model describes the constant temperature systems [2–6,9,11].

### 4.5. Minimal Gaussian constraint model

Let us consider the $N$-particle system with the Hamiltonian

$$H(\mathbf{r},\mathbf{p},a) = \frac{\mathbf{p}^2}{2m} + U(\mathbf{r},a), \tag{57}$$

the function $g(H) = 3N/kT$, and the linear friction

$$\mathbf{F}_i^{(n)} = -\gamma\mathbf{p}_i, \tag{58}$$

where $i = 1,\ldots,N$. Note that $N$ is an arbitrary natural number. Substituting Eq. (58) into Eqs. (15) and (16), we get the power $\mathscr{P}$ and the omega function $\Omega$:

$$\mathscr{P} = -\frac{\gamma}{m}\mathbf{p}^2, \quad \Omega = -3\gamma N.$$

The non-holonomic constraint has the form

$$\frac{\mathbf{p}^2}{m} = kT(a), \tag{59}$$

i.e., the kinetic energy of the system must be a constant. Note that Eq. (59) has not the friction parameter $\gamma$.

For the $N$-particle system with friction (58) and non-holonomic constraint (59), we have the following equations of motion:

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial U}{\partial \mathbf{r}_i} - \gamma\mathbf{p}_i + \lambda\frac{\partial f}{\partial \mathbf{p}_i}, \tag{60}$$

where the function $f$ is defined by

$$f(\mathbf{r},\mathbf{p}) = \tfrac{1}{2}(\mathbf{p}^2 - mkT): \quad f(\mathbf{r},\mathbf{p}) = 0. \tag{61}$$

Eq. (60) and condition (61) define $6N+1$ variables $(\mathbf{r},\mathbf{p},\lambda)$.

Let us find the Lagrange multiplier $\lambda$. Substituting Eq. (61) into Eq. (60), we get

$$\frac{d\mathbf{p}_i}{dt} = -\frac{\partial U}{\partial \mathbf{r}_i} + (\lambda - \gamma)\mathbf{p}_i. \tag{62}$$

Using $df/dt = 0$ in the form

$$\mathbf{p}_i \frac{d\mathbf{p}_i}{dt} = 0 \tag{63}$$

and substituting Eq. (62) into Eq. (63), we get the Lagrange multiplier $\lambda$ in the form

$$\lambda = \frac{1}{mkT}\mathbf{p}_j \frac{\partial U}{\partial \mathbf{r}_j} + \gamma.$$

As a result, we have the holonomic system that is defined by the equations

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = \frac{1}{mkT}\mathbf{p}_i\mathbf{p}_j \frac{\partial U}{\partial \mathbf{r}_j} - \frac{\partial U}{\partial \mathbf{r}_i}. \tag{64}$$

This system is equivalent to the non-holonomic system (60). For the classical $N$-particle system (64), condition (59) is satisfied. If the time evolution of the $N$-particle system is defined by Eq. (64) or Eqs. (60) and (61), then we have the canonical distribution function in the form

$$\rho(\mathbf{r}, \mathbf{p}, a, T) = \exp\frac{1}{kT}(\mathscr{F}(a, T) - H(\mathbf{r}, \mathbf{p}, a)). \tag{65}$$

For example, the $N$-particle system with the forces

$$\mathbf{F}_i = \frac{\omega^2(a)}{kT}\mathbf{p}_i\mathbf{p}_j\mathbf{r}_j - m\omega^2(a)\mathbf{r}_i \tag{66}$$

can have canonical distribution (65) of the linear harmonic oscillator with

$$U(\mathbf{r}, a) = \frac{m\omega^2(a)\mathbf{r}^2}{2}.$$

## 5. Canonical distributions

In this section, we consider the subclass of the canonical non-Hamiltonian system that is described by canonical distribution. This subclass of the canonical non-Hamiltonian $N$-particle system is defined by the simple function $g(H) = 3N\beta(a)$ in the non-holonomic constraint (20).

**Proposition 3.** *If velocity of the elementary phase volume change is directly proportional to the power of non-potential forces, then we have the usual canonical Gibbs distribution as a solution of the Liouville equation.*

In other words, the non-Hamiltonian system with the non-holonomic constraint

$$\Omega = \beta(a)\mathscr{P} \tag{67}$$

can have the canonical Gibbs distribution

$$\rho_N = \exp \beta(a)(\mathscr{F}(a) - H(\mathbf{r}, \mathbf{p}, a))$$

as a solution of the Liouville equation. Here, the coefficient $\beta(a)$ does not depend on $(\mathbf{r}, \mathbf{p}, t)$, i.e.,

$$\mathrm{d}\beta(a)/\mathrm{d}t = 0.$$

For the non-Hamiltonian systems, the omega function (16) does not vanish. Using Eq. (15), we have

$$\Omega = \beta(a)\mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}. \tag{68}$$

In this case, the Liouville equation has the form

$$\frac{\mathrm{d}\rho_N}{\mathrm{d}t} = -\beta(a)\mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i} \rho_N. \tag{69}$$

Let us consider the total time derivative for the Hamiltonian

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t} + \mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}. \tag{70}$$

If $\partial H/\partial t = 0$, then the energy change is equal to the power $\mathscr{P}$ of the non-potential forces $\mathbf{F}_i^{(n)}$. Eq. (69) can be written in the form

$$\frac{\mathrm{d}\rho_N}{\mathrm{d}t} = -\beta(a) \frac{\mathrm{d}H}{\mathrm{d}t} \rho_N. \tag{71}$$

Therefore, the Liouville equation can be rewritten in the form

$$\frac{\mathrm{d} \ln \rho_N(\mathbf{r}, \mathbf{p}, a, t)}{\mathrm{d}t} + \beta(a) \frac{\mathrm{d}H(\mathbf{r}, \mathbf{p}, a)}{\mathrm{d}t} = 0.$$

Since coefficient $\beta(a)$ is a constant ($\mathrm{d}\beta(a)/\mathrm{d}t = 0$), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(\ln \rho_N(\mathbf{r}, \mathbf{p}, a, t) + \beta(a)H(\mathbf{r}, \mathbf{p}, a)) = 0,$$

i.e., the value $(\ln \rho_N + \beta H)$ is a constant along the trajectory of the system in $6N$-dimensional phase space. Let us denote this constant value by $\beta(a)\mathscr{F}(a)$. Then, we have

$$\ln \rho_N(\mathbf{r}, \mathbf{p}, a, t) + \beta(a)H(\mathbf{r}, \mathbf{p}, a) = \beta(a)\mathscr{F}(a),$$

where $\mathrm{d}\mathscr{F}(a)/\mathrm{d}t = 0$. It follows that:

$$\ln \rho_N(\mathbf{r}, \mathbf{p}, a, t) = \beta(a)(\mathscr{F}(a) - H(\mathbf{r}, \mathbf{p}, a)).$$

As a result, we have a canonical distribution function

$$\rho_N(\mathbf{r}, \mathbf{p}, a, t) = \exp \beta(a)(\mathscr{F}(a) - H(\mathbf{r}, \mathbf{p}, a))$$

in the Hamilton picture. The value $\mathscr{F}(a)$ is defined by the normalization condition (40).

Therefore the distribution of this non-Hamiltonian system is a canonical distribution.

Note that $N$ is an arbitrary natural number since we do not use the condition $N \gg 1$ or $N \to \infty$.

## 6. Non-canonical distributions

The well-known non-Gaussian distribution is the Breit–Wigner distribution. This distribution has a probability density function in the form

$$\rho(x) = \frac{1}{\pi(1+x^2)}. \tag{72}$$

The Breit–Wigner distribution is also known in statistics as Cauchy distribution. The Breit–Wigner distribution is a generalized form originally introduced [28] to describe the cross-section of resonant nuclear scattering in the form

$$\rho(H) = \frac{\lambda}{(H-E)^2 + (\Gamma/2)^2}. \tag{73}$$

This distribution can be derived from the transition probability of a resonant state with known lifetime [29–31].

If the function $g(H)$ of the non-holonomic constrain is defined by

$$g(H) = \frac{2(H-E)}{(H-E)^2 + (\Gamma/2)^2}, \tag{74}$$

then we have non-Hamiltonian systems with the Breit–Wigner distribution as a solution of the Liouville equation.

If the function $g(H)$ of the non-holonomic constrain has the form

$$g(H) = \frac{\beta(a)}{1 + \alpha \exp \beta(a) H}, \tag{75}$$

then we have classical non-Hamiltonian systems with Fermi–Bose distribution (12) considered by Ebeling [13]. This distribution can be derived as a solution of the Liouville equation. Note that Ebeling derives the Fermi–Bose distribution function as a solution of the Fokker–Planck equation. It is known that Fokker–Planck equation can be derived from the Liouville equation [14].

If the non-potential forces $\mathbf{F}_i^{(n)}$ are determined by the Hamiltonian

$$\mathbf{F}_i^{(n)} = -\partial G(H)/\partial \mathbf{p}_i, \tag{76}$$

then we have the canonical non-Hamiltonian systems, which are considered in [12,13]. These systems are called canonical dissipative systems.

Note that the linear function $g(H)$ in the form

$$g(H) = \beta_1(a) + \beta_2(a) H$$

leads to the following non-canonical distribution function:

$$\rho_N = Z(a) \exp -(\beta_1(a) H + \tfrac{1}{2}\beta_2(a) H^2). \tag{77}$$

The proof of this proposition can be directly derived from Eqs. (32) and (30).

Let us assume that Eq. (11) can be solved in the form

$$H = \theta(a)h(\rho_N), \tag{78}$$

where $h$ depends on the distribution $\rho_N$. The function $\theta(a)$ is a function of the parameters $a$. In this case, the function $g(H)$ is a composite function

$$R(\rho_N) = -g(\theta(a)h(\rho_N)). \tag{79}$$

This function can be defined by

$$R(\rho_N) = \frac{1}{\rho_N}\left(\theta(a)\frac{\partial h(\rho_N)}{\partial \rho_N}\right)^{-1}. \tag{80}$$

In this case, the Liouville equation for the non-Hamiltonian system has the form

$$\frac{\mathrm{d}\rho_N}{\mathrm{d}t} = R(\rho_N)\mathscr{P}. \tag{81}$$

This equation is a non-linear equation. Note that the classical Fermi–Bose systems [13] have the function in the form

$$R(\rho_N) = -\beta(a)(\rho_N - s\rho_N^2). \tag{82}$$

The non-linearity of the Liouville equation is not connected with an incorrectly defined phase space. This non-linearity is a symptom of the use of an incorrectly defined boundary condition. The Bogoliubov principle of correlation weakening cannot be used for classical Fermi–Bose systems. The classical Fermi–Bose systems can be considered as a model of open (non-Hamiltonian) system with the special correlation. Note that the non-linear evolution of statistical systems is considered in [33–39].

## 7. Thermodynamics laws for non-Hamiltonian systems

Let us define the mean value $f(a)$ of the function $f(\mathbf{r},\mathbf{p},a)$ by the relation

$$f(a) = \int f(\mathbf{r},\mathbf{p},a)\rho_N(\mathbf{r},\mathbf{p},a)\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p} \tag{83}$$

and the variation for this function by

$$\delta_a f(\mathbf{r},\mathbf{p},a) = \sum_{k=1}^{n} \frac{\partial f(\mathbf{r},\mathbf{p},a)}{\partial a_k}\,\mathrm{d}a_k. \tag{84}$$

The first law of thermodynamic states that the internal energy $U(a)$ may change because of heat transfer $\delta Q$, and work of thermodynamic forces

$$\delta A = \sum_{k=1}^{n} F_k(a)\,\mathrm{d}a_k. \tag{85}$$

The external parameters $a = \{a_1,a_2,\ldots,a_n\}$ here act as generalized coordinates. In the usual equilibrium thermodynamics the work done does not entirely account for the change in the internal energy. The internal energy also changes because of the transfer of heat, and so

$$\mathrm{d}U = \delta Q - \delta A. \tag{86}$$

Since thermodynamic forces $F_k(a)$ are non-potential forces

$$\frac{\partial F_k(a)}{\partial a_l} = \frac{\partial F_l(a)}{\partial a_k}, \tag{87}$$

the amount of work $\delta A$ depends on the path of transition from one state in parameters space to another. For this reason $\delta A$ and $\delta Q$, taken separately, are not total differentials.

Let us give a statistical definition of thermodynamic forces for the non-Hamiltonian systems in the mathematical expression of the analog of the first thermodynamics law for the mean values. It would be natural to define the internal energy as the mean value of Hamiltonian

$$U(a) = \int H(\mathbf{r},\mathbf{p},a)\rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p}. \tag{88}$$

It follows that the expression for the total differential has the form:

$$\mathrm{d}U(a) = \int \delta_a H(\mathbf{r},\mathbf{p},a)\rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p} + \int H(\mathbf{r},\mathbf{p},a)\delta_a\rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p}.$$

Therefore

$$\begin{aligned}\mathrm{d}U(a) = &\int \frac{\partial H(\mathbf{r},\mathbf{p},a)}{\partial a_k}\delta a_k\rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p} \\ &+ \int H(\mathbf{r},\mathbf{p},a)\delta_a\rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p}.\end{aligned} \tag{89}$$

In the first term on the right-hand side, we can use the definition of phase density of the thermodynamic force

$$F_k^{\mathrm{ph}}(\mathbf{r},\mathbf{p},a) = -\frac{\partial H(\mathbf{r},\mathbf{p},a)}{\partial a_k}.$$

The thermodynamic force $F_k(a)$ is a mean value of the phase density of the thermodynamic force

$$F_k(a) = \int F_k^{\mathrm{ph}}(\mathbf{r},\mathbf{p},a)\rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p}. \tag{90}$$

Using this equation we can prove the relation (87).

Analyzing these expressions we see that the first term on the right-hand side of Eq. (89) answers for the work (85) of thermodynamic forces (90), whereas the amount of the heat transfer is given by

$$\delta Q = \int H(\mathbf{r},\mathbf{p},a)\delta_a\rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p}. \tag{91}$$

We see that the heat transfer term accounts for the change in the internal energy due not to the work of thermodynamic forces, but rather to change in the distribution function cased by the external parameters $a$.

Now let us turn our attention to the analog of the second law for the non-Hamiltonian systems.

The second law of thermodynamics has the form

$$\delta Q = \theta(a)\,\mathrm{d}S(a). \tag{92}$$

This implies that there exists a function of state $S(a)$ called entropy. The function $\theta(a)$ acts as integration factor.

Let us prove that (92) follows from the statistical definition of $\delta Q$ in Eq. (91). For Eq. (91), we take the distribution that is defined by the Hamiltonian, and show that (91) can be reduced to (92).

Let us assume that Eq. (11) can be solved in the form

$$H = \theta(a)h(\rho_N),$$

where $h$ depends on the distribution $\rho_N$. The function $\theta(a)$ is a function of the parameters $a = \{a_1, a_2, \ldots, a_n\}$.

We rewrite (91) in the equivalent form

$$\delta Q = \int (\theta(a)\,h(\rho(\mathbf{r},\mathbf{p},a),a) + C(a))\,\delta_a \rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p}. \tag{93}$$

New term with $C(a)$, which is added into this equation, is equal to zero because of the normalization condition of the distribution function $\rho_N$

$$C(a)\delta_a \int \rho_N(\mathbf{r},\mathbf{p},a)\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p} = C(a)\delta_a 1 = 0.$$

We can write Eq. (93) in the form

$$\delta Q = \theta(a)\delta_a \int K(\rho_N(\mathbf{r},\mathbf{p},a))\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p}, \tag{94}$$

where the function $K = K(\rho_N)$ is defined by

$$\frac{\partial K(\rho_N)}{\partial \rho_N} = h(\rho_N) + C(a)/\theta(a). \tag{95}$$

We see that the expression for $\delta Q$ is integrable. If we take $1/\theta(a)$ for the integration factor, thus identifying $\theta(a)$ with the analog of absolute temperature, then, using (92) and (94), we can give the statistical definition of entropy

$$S(a) = \int\int K(\rho_N(\mathbf{r},\mathbf{p},a))\,\mathrm{d}^N\mathbf{r}\,\mathrm{d}^N\mathbf{p} + S_0. \tag{96}$$

Here, $S_0$ is the contribution to the entropy which does not depend on the variables $a$, but may depend on the number of particles $N$ in the system. Note that the expression for entropy is equivalent to the mean value of phase density function

$$S^{\mathrm{ph}}(\mathbf{r},\mathbf{p},a) = K(\rho_N(\mathbf{r},\mathbf{p},a))/\rho_N(\mathbf{r},\mathbf{p},a) + C(a). \tag{97}$$

$S^{\rm ph}$ is a function of dynamic variables $\mathbf{r}$, $\mathbf{p}$, and the parameters $a = \{a_1, a_2, \ldots, a_n\}$. The number $N$ is an arbitrary natural number since we do not use the condition $N \gg 1$ or $N \to \infty$. Note that in the usual equilibrium thermodynamics the function $\theta(a)$ is a mean value of kinetic energy. In the suggested thermodynamics for the non-Hamiltonian systems $\theta(a)$ is the usual function of the external parameters $a = \{a_1, a_2, \ldots, a_n\}$.

## 8. Conclusion

The aim of this paper was the extension of the statistical mechanics of conservative Hamiltonian systems to non-Hamiltonian and dissipative systems. In this paper, we consider a wide class of non-Hamiltonian statistical systems that have (canonical or non-canonical) distributions that are defined by Hamiltonian. This class can be described by the non-holonomic (non-integrable) constraint: the velocity of the elementary phase volume change is directly proportional to the power of non-potential forces. The coefficient of this proportionality is defined by Hamiltonian. The special constraint allows us to derive solution for the distribution function of the system, even in far-from equilibrium situation. These distributions, which are defined by Hamiltonian, can be derived analytically as solutions of the Liouville equation for non-Hamiltonian systems.

The suggested class of the non-Hamiltonian systems is characterized by the distribution functions that are determined by the Hamiltonian. The constant temperature systems [2–6,9], the canonical–dissipative systems [12,13], and the Fermi–Bose classical systems [13] are the special cases of suggested class of non-Hamiltonian systems. For the non-Hamiltonian $N$-particle systems of this class, we can use the analogs of the usual thermodynamics laws. Note that $N$ is an arbitrary natural number since we do not use the condition $N \gg 1$ or $N \to \infty$. This allows us to use the suggested class of non-Hamiltonian systems for the simulation schemes [32] for the molecular dynamics.

In the papers [40–42], the quantization of the evolution equations for non-Hamiltonian and dissipative systems was suggested. Using this quantization it is easy to derive the quantum Liouville–von Neumann equations for the $N$-particle statistical operator of the non-Hamiltonian quantum system [26]. We can derive the canonical and non-canonical statistical operators that are determined by the Hamiltonian [17,18]. The condition for non-Hamiltonian systems can be generalized by the quantization method suggested in [40,41].

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