Canonical Gibbs Distribution for Dissipative Systems

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Abstract

A class of non-Hamiltonian and dissipative systems that have canonical distribution determined by Hamiltonian is described. The distributions are derived as stationary solutions of the Liouville equation which expresses conservation of probability in a phase space of dissipative systems. The class of dissipative 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.

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 which act on particles are the sum of potential and non-potential forces. It is natural to ask if a canonical distribution for non-Hamiltonian and dissipative systems exist? This type of questions are timely due to the interest in generalizations of statistical mechanics, for example, the non-Hamiltonian statistical mechanics [2, 3, 4, 5, 6, 7] and the fractional statistical mechanics [8, 6]. Quantum dissipative and non-Hamiltonian systems can have the same distributions as Hamiltonian systems [7]. The canonical distribution for simple non-Hamiltonian and dissipative systems is considered in Refs. [9, 10, 11, 12, 13, 14, 5]. Note that the system which is a nondissipative system in the usual phase space, can be a dissipative system in the fractional phase space [6].

The aim of this work is the extension of the statistical mechanics of conservative Hamiltonian systems to the non-Hamiltonian and dissipative systems. In this paper we describe a wide class of non-Hamiltonian and dissipative systems that have canonical distribution defined by Hamiltonian. This class can be described by the non-holonomic (non-integrable) constraint [5]: the velocity of the elementary phase volume change must be directly proportional to the power of non-potential forces. These distributions are derived analytically as solutions of the Liouville equation which express the conservation of probability in the phase space of non-Hamiltonian systems. The special constraint allows in many cases derive solution even in far-from-equilibrium states. The non-Hamiltonian systems with minimal Gaussian constraint [9, 10, 11, 12, 13, 14] which can be described by the isokinetic thermostat are the special cases of suggested class of non-Hamiltonian and dissipative systems.

2 Non-Hamiltonian and Dissipative Systems

Let us consider the definitions of non-Hamiltonian and dissipative classical systems [15], which are used for the formulation of our results.

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 $i = 1, ..., N$, 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.
A mechanical system is called non-Hamiltonian if at least one of conditions (2) is not satisfied.

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

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \tag{3}$$

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 nonlinear one-dimensional sigma-model [18] the second term of the left-hand side of Eq. (5) is defined by the metric.

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

$$\int \rho_N(q_t, p_t, a, t) d^N q_t d^N p_t = 1. \tag{6}$$

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

$$\frac{d\rho_N(q_t, p_t, a, t)}{dt} = -\Omega(q_t, p_t, a, t)\rho_N(q_t, p_t, a, t). \tag{7}$$

This equation describes the change of the distribution function ρ_N along the trajectory in the 6N-dimensional phase space. Here Ω 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 d/dt is a total time derivative:

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

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 nonlinear one-dimensional sigma-model [18]

In the Liouville picture (for the Lagrange variables) the function Ω defines the velocity of the phase volume change [16]:

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

Definition 2. *If $\Omega \leq 0$ 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

$$S(q_t, p_t, a, t) = -k \; ln \; \rho_N(q_t, p_t, a, t).$$

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

$$\frac{dS(q_t, p_t, a, t)}{dt} = k\Omega(q_t, p_t, a, t). \tag{10}$$

It is easy to see that the function Ω is proportional to the velocity of the phase entropy density change. Therefore, the dissipative systems can be defined by the following equivalent definition: *A system is called a generalized dissipative system if the velocity of the entropy density change does not equal to zero.*

3 Distributions as Solution of the Liouville Equation

Let us formulate the proposition which allows one to answer the following question: Can a non-Hamiltonian system have a canonical Gibbs distribution?

Let us consider the N-particle non-Hamiltonian system (1), where $\mathbf{G}_i$ are determined by the Hamiltonian $H(\mathbf{q},\mathbf{p},a)$

$$G_i = \frac{\partial H}{\partial \mathbf{p}_i} \tag{11}$$

and the function $H = H(\mathbf{q},\mathbf{p},a)$ is a smooth function on the momentum space. In general, we can write the forces $\mathbf{F}_i$ in the form

$$\mathbf{F}_i = -\frac{\partial H}{\partial \mathbf{q}_i} + \mathbf{F}_i^{(n)}, \tag{12}$$

where $\mathbf{F}_i^{(n)}$ is the sum of non-potential forces (internal and external), which act on the ith particle.

In this case the non-Hamiltonian system is defined by the equations

$$\frac{d\mathbf{q}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial H}{\partial \mathbf{q}_i} + \mathbf{F}_i^{(n)}. \tag{13}$$

The power of non-potential forces $\mathcal{P}$ is defined by

$$\mathcal{P}(\mathbf{q},\mathbf{p},t) = \mathbf{F}_i^{(n)}\mathbf{v}_i, \quad where \quad \mathbf{v}_i = \frac{\partial H}{\partial \mathbf{p}_i}. \tag{14}$$

The velocity of an elementary phase volume change Ω is defined by the relation

$$\Omega(\mathbf{q},\mathbf{p},t) = \frac{\partial \mathbf{F}_i^{(n)}}{\partial \mathbf{p}_i} + \frac{\partial^2 H}{\partial \mathbf{q}_i \partial \mathbf{p}_i}. \tag{15}$$

Proposition 1. *If velocity of the elementary phase volume change Ω is directly proportional to the power $\mathcal{P}$ of non-potential forces $\mathbf{F}_i^{(n)}$ of the non-Hamiltonian system (13) and coefficient of this proportionality is a function $\beta(a)$ of the external parameters*

$$\Omega(\mathbf{q},\mathbf{p},t) - \beta(a)\mathcal{P}(\mathbf{q},\mathbf{p},t) = 0, \tag{16}$$

i.e., non-potential forces $\mathbf{F}_i^{(n)}$ of the non-Hamiltonian system (13) satisfy the constraint condition

$$\beta(a)\mathbf{F}_i^{(n)}\frac{\partial H}{\partial \mathbf{p}_i} - \frac{\partial \mathbf{F}_i^{(n)}}{\partial \mathbf{p}_i} - \frac{\partial^2 H}{\partial \mathbf{q}_i \partial \mathbf{p}_i} = 0, \tag{17}$$

then this non-Hamiltonian system has canonical Gibbs distribution.

$$\rho_N(\mathbf{q},\mathbf{p},a,t) = exp\beta(a)\Big(\mathcal{F}(a) - H(\mathbf{q},\mathbf{p},a)\Big), \tag{18}$$

where $\mathcal{F}(a)$ is defined by normalization condition (6).

Any non-Hamiltonian system with the non-holonomic constraint for the non-potential forces (17) have canonical distribution.

Proof

Let us prove that canonical distributions defined by the Hamiltonian can be derived as solutions of the Liouville equation with the non-holonomic constraint.

Let us consider the Liouville equation for the N-particle distribution function $\rho_N = \rho_N(\mathbf{q}, \mathbf{p}, t)$. The Liouville equation for this non-Hamiltonian system

$$\frac{\partial \rho_N}{\partial t} + \frac{\partial}{\partial \mathbf{q}_i}\Big(\mathbf{G}_i \rho_N\Big) + \frac{\partial}{\partial \mathbf{p}_i}\Big(\mathbf{F}_i \rho_N\Big) = 0 \tag{19}$$

expresses the conservation of probability in the phase space. If we define a total time derivative along the phase space trajectory by (9), then the Liouville equation (19) can be written in the form (7). In classical mechanics of Hamiltonian systems the right-hand side of this equation is zero, and the distribution function does not change in time evolution. Let us assume that velocity of the entropy density change $\Omega(\mathbf{q}_t, \mathbf{p}_t, a, t)$ is directly proportional to the power $\mathcal{P}(\mathbf{q}_t, \mathbf{p}_t, a, t)$ of the non-potential forces:

$$\Omega(\mathbf{q}_t, \mathbf{p}_t, a, t) = \beta(a)\mathcal{P}(\mathbf{q}_t, \mathbf{p}_t, a, t), \tag{20}$$

with some coefficient $\beta(a)$ which does not depend on $(\mathbf{q}_t, \mathbf{p}_t, t)$, i.e. $d\beta(a)/dt = 0$.

For the non-Hamiltonian systems, the omega function (8) does not vanish. Using the constraint (16) for the non-Hamiltonian and dissipative systems, this function is defined by

$$\Omega = \beta(a)\mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}. \tag{21}$$

In this case, the Liouville equation has the form

$$\frac{d\rho_N}{dt} = -\beta(a)\mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}\rho_N. \tag{22}$$

Let us consider the total time derivative for the Hamilton function

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \mathbf{G}_i \frac{\partial H}{\partial \mathbf{q}_i} + \mathbf{F}_i \frac{\partial H}{\partial \mathbf{p}_i} = \frac{\partial H}{\partial t} + \frac{\partial H}{\partial \mathbf{p}_i}\frac{\partial H}{\partial \mathbf{q}_i} + \Big(-\frac{\partial H}{\partial \mathbf{q}_i} + \mathbf{F}_i^{(n)}\Big)\frac{\partial H}{\partial \mathbf{p}_i}$$

Hence

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \mathbf{F}_i^{(n)} \frac{\partial H}{\partial \mathbf{p}_i}. \tag{23}$$

If $\partial H/\partial t = 0$, then the energy change is equal to the power $\mathcal{P}$ of the non-potential forces $\mathbf{F}_i^{(n)}$ and we have $\Omega = \beta(a)dH/dt$. The Liouville equation can be written in the form

$$\frac{d\rho_N}{dt} = -\beta(a)\frac{dH}{dt}\rho_N. \tag{24}$$

Therefore, the Liouville equation can be rewritten in the form

$$\frac{d\ ln\rho_N(\mathbf{q}_t, \mathbf{p}_t, a, t)}{dt} + \beta(a)\frac{dH(\mathbf{q}_t, \mathbf{p}_t, a)}{dt} = 0.$$

Since coefficient $\beta(a)$ is a constant, we have

$$\frac{d}{dt}\Big(ln\rho_N(\mathbf{q}_t, \mathbf{p}_t, a, t) + \beta(a)H(\mathbf{q}_t, \mathbf{p}_t, a)\Big) = 0,$$

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 $\beta(a)\mathcal{F}(a)$. Then we have

$$ln\rho_N(\mathbf{q}_t, \mathbf{p}_t, a, t) + \beta(a)H(\mathbf{q}_t, \mathbf{p}_t, a) = \beta(a)\mathcal{F}(a),$$

where $d\mathcal{F}(a)/dt = 0$, i.e.

$$ln\ \rho_N(\mathbf{q}_t, \mathbf{p}_t, a, t) = \beta(a)\Big(\mathcal{F}(a) - H(\mathbf{q}_t, \mathbf{p}_t, a)\Big).$$

As a result we have a canonical distribution function

$$\rho_N(\mathbf{q}_t, \mathbf{p}_t, a, t) = exp\beta(a)\Big(\mathcal{F}(a) - H(\mathbf{q}_t, \mathbf{p}_t, a)\Big)$$

in the Hamilton picture. The function $\mathcal{F}(a)$ is defined by normalization condition (30).

Therefore, the distribution of this non-Hamiltonian system is canonical distribution

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

4 Non-Holonomic Constraint for Non-Hamiltonian Systems

Let us formulate the proposition which allows one to derive the non-Hamiltonian systems with canonical distributions using any non-Hamiltonian systems.

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

$$\frac{d\mathbf{q}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i, \tag{25}$$

where $\mathbf{F}_i$ is the sum of potential and non-potential forces, there exists a non-Hamiltonian system with canonical distribution ρ_N defined by the equation

$$\frac{d\mathbf{q}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i^{new}, \tag{26}$$

where the new non-potential forces are defined by

$$\mathbf{F}_i^{new} = \frac{\mathbf{P}_k\mathbf{P}_k\delta_{ij} - \mathbf{P}_i\mathbf{P}_j}{\mathbf{P}_k\mathbf{P}_k}\mathbf{F}_j - \frac{\mathbf{P}_i\mathbf{Q}_j}{\mathbf{P}_k\mathbf{P}_k}\frac{\partial H}{\partial \mathbf{p}_j}. \tag{27}$$

Here

$$\mathbf{P}_i = \beta(a)\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_i}\frac{\partial H}{\partial \mathbf{p}_j} + \beta(a)\mathbf{F}_j^{(n)}\frac{\partial^2 H}{\partial \mathbf{p}_i \partial \mathbf{p}_j} - \frac{\partial^2 \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_i \partial \mathbf{p}_j} - \frac{\partial^3 H}{\partial \mathbf{p}_i \partial \mathbf{q}_j \partial \mathbf{p}_j}, \tag{28}$$

and

$$\mathbf{Q}_i = \beta(a)\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{q}_i}\frac{\partial H}{\partial \mathbf{p}_j} + \beta(a)\mathbf{F}_j^{(n)}\frac{\partial^2 H}{\partial \mathbf{q}_i \partial \mathbf{p}_j} - \frac{\partial^2 \mathbf{F}_j^{(n)}}{\partial \mathbf{q}_i \partial \mathbf{p}_j} - \frac{\partial^3 H}{\partial \mathbf{q}_i \partial \mathbf{q}_j \partial \mathbf{p}_j}. \tag{29}$$

Note that the forces defined by Eq. (27) satisfy the condition (17). This is easy to prove by direct calculation.

Proof.

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

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

$$f(\mathbf{q},\mathbf{p})=0. \tag{30}$$

Differentiation of Eq. (30) with respect to time gives a relation

$$\mathbf{P}_i(\mathbf{q},\mathbf{p})\frac{d\mathbf{p_i}}{dt}+\mathbf{Q}_i(\mathbf{q},\mathbf{p})\frac{d\mathbf{r_i}}{dt}=0, \tag{31}$$

where

$$\mathbf{P}_i(\mathbf{q},\mathbf{p})=\frac{\partial f}{\partial \mathbf{p}_i},\quad \mathbf{Q}_i(\mathbf{q},\mathbf{p})=\frac{\partial f}{\partial \mathbf{q}_i}. \tag{32}$$

An unconstrained motion of the ith particle, where $i=1,...,N$, is described by the equations

$$\frac{d\mathbf{q}_i}{dt}=\mathbf{G}_i,\quad \frac{d\mathbf{p}_i}{dt}=\mathbf{F}_i, \tag{33}$$

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

The unconstrained motion gives a trajectory which leaves the constraint hypersurface defined by Eq. (30). The constraint forces $\mathbf{R}_i$ must be added to the equation of motion to prevent the deviation from the constraint hypersurface:

$$\frac{d\mathbf{q}_i}{dt}=\mathbf{G}_i,\quad \frac{d\mathbf{p}_i}{dt}=\mathbf{F}_i+\mathbf{R}_i. \tag{34}$$

The constraint force $\mathbf{R}_i$ for the non-holonomic constraint is proportional to $\mathbf{P}_i$

$$\mathbf{R}_i=\lambda\mathbf{P}_i, \tag{35}$$

where the coefficient λ of the constraint force term is an undetermined Lagrangian multiplier. For the non-holonomic constraint (30) the equations of motion (33) are modified as

$$\frac{d\mathbf{q}_i}{dt}=\mathbf{G}_i,\quad \frac{d\mathbf{p}_i}{dt}=\mathbf{F}_i+\lambda\mathbf{P}_i. \tag{36}$$

The Lagrangian coefficient is determined to satisfy the time derivative of the constraint equation (31). Substituting Eq. (34) into Eq. (31), we get

$$\mathbf{P}_i(\mathbf{F}_i+\lambda\mathbf{P}_i)+\mathbf{Q}_i\mathbf{G}_i=0. \tag{37}$$

Therefore, we have that the Lagrange multiplier λ is equal to

$$\lambda=-\frac{\mathbf{P}_i\mathbf{F}_i+\mathbf{Q}_i\mathbf{G}_i}{\mathbf{P}_k\mathbf{P}_k}. \tag{38}$$

As a result, we obtain the following equations

$$\frac{d\mathbf{q}_i}{dt}=\mathbf{G}_i,\quad \frac{d\mathbf{p}_i}{dt}=\mathbf{F}_i-\mathbf{P}_i\frac{\mathbf{P}_j\mathbf{F}_j+\mathbf{Q}_j\mathbf{G}_j}{\mathbf{P}_k\mathbf{P}_k}. \tag{39}$$

These equations we can rewrite in the form

$$\frac{d\mathbf{q}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i^{new} \tag{40}$$

with the new forces

$$\mathbf{F}_i^{new} = \frac{\mathbf{P}_k \mathbf{P}_k \delta_{ij} - \mathbf{P}_i \mathbf{P}_j}{\mathbf{P}_k \mathbf{P}_k} \mathbf{F}_j - \frac{\mathbf{P}_i \mathbf{Q}_j}{\mathbf{P}_k \mathbf{P}_k} \mathbf{G}_j. \tag{41}$$

In general, the forces $\mathbf{F}_i^{new}$ are non-potentials forces.

Eqs. (39) or (41) are equations of the *holonomic* non-Hamiltonian system with n degrees of freedom. For any trajectory of the system in the phase space, we have $f = const$. If initial values $\mathbf{q}_k(0)$ and $\mathbf{p}_k(0)$ satisfy the constraint condition $f(\mathbf{q}(0), \mathbf{p}(0), t_0) = 0$, then solution of Eqs. (39) and (41) is a motion of the non-holonomic system.

Let us consider the non-Hamiltonian system with

$$\mathbf{G}_i = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \mathbf{F}_i = -\frac{\partial H}{\partial \mathbf{q}_i} + \mathbf{F}_i^{(n)}, \tag{42}$$

and the special form of the non-holonomic constraint (30). Let us assume that the velocity of the elementary phase volume change $\Omega(\mathbf{q}_t, \mathbf{p}_t, a, t)$ is directly proportional to the power $\mathcal{P}(\mathbf{q}_t, \mathbf{p}_t, a, t)$ of the non-potential forces. The power $\mathcal{P}$ of the non-potential forces $\mathbf{F}_i^{(n)}$ is defined by Eq. (14). The omega function Ω is defined by Eq. (15). Therefore, the system is subject to a non-holonomic (non-integrable) constraint in the form

$$f(\mathbf{q}_t, \mathbf{p}_t, a) = \beta(a)\mathcal{P}(\mathbf{q}_t, \mathbf{p}_t, a) - \Omega(\mathbf{q}_t, \mathbf{p}_t, a) = 0. \tag{43}$$

This equation for the non-potential forces has the form

$$\beta(a)\mathbf{F}_j^{(n)} \frac{\partial H}{\partial \mathbf{p}_j} - \frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_j} - \frac{\partial^2 H}{\partial \mathbf{q}_j \partial \mathbf{p}_j} = 0. \tag{44}$$

Let us find $\mathbf{P}_i$ and $\mathbf{Q}_i$ for this constraint. Using (28), differentiation of the function $f(\mathbf{q}_t, \mathbf{p}_t, t)$ with respect to $\mathbf{p}_i$ gives

$$\mathbf{P}_i = \frac{\partial f}{\partial \mathbf{p}_i} = \frac{\partial}{\partial \mathbf{p}_i}\Big(\beta(a)\mathbf{F}_j^{(n)} \frac{\partial H}{\partial \mathbf{p}_j}\Big) - \frac{\partial}{\partial \mathbf{p}_i}\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_j} - \frac{\partial}{\partial \mathbf{p}_i}\frac{\partial^2 H}{\partial \mathbf{q}_j \partial \mathbf{p}_j}. \tag{45}$$

Differentiation of function $f(\mathbf{q}_t, \mathbf{p}_t, t)$ with respect to $\mathbf{q}_i$ gives

$$\mathbf{Q}_i = \frac{\partial f}{\partial \mathbf{q}_i} = \frac{\partial}{\partial \mathbf{q}_i}\Big(\beta(a)\mathbf{F}_j^{(n)} \frac{\partial H}{\partial \mathbf{p}_j}\Big) - \frac{\partial}{\partial \mathbf{q}_i}\frac{\partial \mathbf{F}_j^{(n)}}{\partial \mathbf{p}_j} - \frac{\partial}{\partial \mathbf{q}_i}\frac{\partial^2 H}{\partial \mathbf{q}_j \partial \mathbf{p}_j}. \tag{46}$$

5 Dissipative System with Gaussian Constraint

Let us consider the N-particle system with the Hamiltonian

$$H(\mathbf{q}, \mathbf{p}, a) = \frac{\mathbf{p}_i^2}{2m} + U(\mathbf{q}, a), \tag{47}$$

the function $\beta(a) = 3N/kT(a)$, and a linear friction defined by non-potential forces

$$\mathbf{F}_i^{(n)} = -\gamma \mathbf{p}_i, \tag{48}$$

where $i = 1, ..., N$. Note that N is an arbitrary natural number. Substituting Eq. (48) into Eqs. (14) and (15), we get the power $\mathcal{P}$ and the Gibbs phase Ω:

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

The non-holonomic constraint has the form

$$\frac{\mathbf{p}_i^2}{m} = kT(a), \tag{49}$$

i.e., the kinetic energy of the system must be a constant. Note that Eq. (49) has no friction parameter γ.

The equations of motion for the N-particle system with friction (48) and non-holonomic constraint (51) have the form

$$\frac{d\mathbf{q}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial U}{\partial \mathbf{q}_i} - \gamma \mathbf{p}_i + \lambda \frac{\partial f}{\partial \mathbf{p}_i}, \tag{50}$$

where the function f is defined by

$$f(\mathbf{q}, \mathbf{p}) = \frac{1}{2}\Big(\mathbf{p}_i^2 - mkT\Big) : \quad f(\mathbf{q}, \mathbf{p}) = 0. \tag{51}$$

Eqs. (50) with condition (51) define 6N+1 variables $(\mathbf{q}, \mathbf{p}, \lambda)$.

It is easy to find the functions

$$\mathbf{P}_i = \frac{\partial f}{\partial \mathbf{p}_i} = \mathbf{p}_i, \quad \mathbf{Q}_i = \frac{\partial f}{\partial \mathbf{q}_i} = 0. \tag{52}$$

As a result, we have the holonomic system which is equivalent to the non-holonomic system (50), (51) and is defined by

$$\frac{d\mathbf{q}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial U}{\partial \mathbf{q}_j}\Big(\delta_{ij} - \frac{\mathbf{p}_i\mathbf{p}_j}{\mathbf{p}^2}\Big). \tag{53}$$

Here we can use Eq. (49) to derive the equations of motion in the form

$$\frac{d\mathbf{q}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = \frac{1}{mkT}\mathbf{p}_i\mathbf{p}_j\frac{\partial U}{\partial \mathbf{q}_j} - \frac{\partial U}{\partial \mathbf{q}_i}. \tag{54}$$

Condition (49) for the classical N-particle system (54) is satisfied. If the time evolution of the N-particle system is defined by Eq. (54) or Eqs. (50) and (51), then we have the canonical distribution function in the form

$$\rho(\mathbf{q}, \mathbf{p}, a, T) = exp\frac{1}{kT}\Big(\mathcal{F}(a, T) - H(\mathbf{q}, \mathbf{p}, a)\Big). \tag{55}$$

For example, the N-particle system with the forces

$$\mathbf{F}_i = \frac{\omega^2(a)}{kT}\mathbf{p}_i\mathbf{p}_j\mathbf{q}_j - m\omega^2(a)\mathbf{q}_i \tag{56}$$

can have a canonical distribution which looks like the canonical distribution (55) of the linear harmonic oscillator, where

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

6 Conclusion

The aim of this work is the extension of the statistical mechanics of conservative Hamiltonian systems to the non-Hamiltonian and dissipative systems. In this paper we consider a wide class of non-Hamiltonian statistical systems that have canonical distribution defined by a Hamiltonian.

In the paper [5], the canonical distribution is considered as a stationary solution of the Liouville equation for a wide class of classical 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 (phase entropy density) change. This constraint is a non-holonomic constraint which leads to the canonical distribution as a stationary solution of the Liouville equations. In a simple case we derived the constant temperature systems which are defined by minimum Gaussian constraint. These systems [9, 10, 11, 12, 13, 14] are the special cases of the 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 $N >> 1$ or $N \to \infty$. This allows one to use the suggested class of non-Hamiltonian and dissipative systems for the simulation schemes [17] for the molecular dynamics.

In the papers [19, 20, 21], quantization of the evolution equations for non-Hamiltonian and dissipative systems was suggested. Using this quantization it is easy to derive quantum Liouville-von Neumann equations for the N-particle statistical operator of the non-Hamiltonian quantum system [16]. The condition which leads to the canonical and non-canonical statistical operators determined by the Hamiltonian [7] can be generalized for the quantum case by the quantization method suggested in [19, 20].

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