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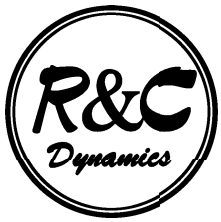

CANONICAL GIBBS DISTRIBUTION AND THERMODYNAMICS OF MECHANICAL SYSTEMS WITH A FINITE NUMBER OF DEGREES OF FREEDOM

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Traditional derivation of Gibbs canonical distribution and the justification of thermodynamics are based on the assumption concerning an isoenergetic ergodicity of a system of n weakly interacting identical subsystems and passage to the limit $n \to \infty$. In the presented work we develop another approach to these problems assuming that n is fixed and $n \geqslant 2$. The ergodic hypothesis (which frequently is not valid due to known results of the KAM-theory) is substituted by a weaker assumption that the perturbed system does not have additional first integrals independent of the energy integral. The proof of nonintegrability of perturbed Hamiltonian systems is based on the Poincaré method. Moreover, we use the natural Gibbs assumption concerning a thermodynamic equilibrium of subsystems at vanishing interaction. The general results are applied to the system of the weakly connected pendula. The averaging with respect to the Gibbs measure allows to pass from usual dynamics of mechanical systems to the classical thermodynamic model.

1. Introduction

The classical approach to the justification of thermodynamics is based on the use of *Gibbs canonical distribution*

$$\rho(x,y) = \frac{e^{-\beta H}}{\int e^{-\beta H}\,dx\,dy}\,. \tag{1.1}$$

Here x and y are canonical coordinates and momenta respectively, $H(x,y)$ is the Hamiltonian function of a mechanical system, $\beta = \text{const}$. The function ρ is treated as a stationary density of probability distribution. More precisely, we suppose that the system in the given state is a random event, and the probability of detection of the system in area D of the phase space is equal to

$$\int\limits_D \rho(x,y)\,dx\,dy\,.$$

The parameter β is determined from the equality

$$E = \int H\rho\,dx\,dy\,, \tag{1.2}$$

where E is average energy of the system. Usually this parameter is supposed to be $\beta = \frac{1}{kT}$, where T is the absolute temperature, k is the Boltzmann constant [1]–[4]. We assume that the integrals (1.1) and (1.2), extended to the whole phase space, are converging.

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The justification of Gibbs distribution is one of basic problems of statistical mechanics. For this purpose one usually considers N *indistinguishable* systems with the Hamiltonians

$$H(x^{(\alpha)}, y^{(\alpha)}), \qquad \alpha = 1, \dots, N, \tag{1.3}$$

where $x^{(\alpha)}$, $y^{(\alpha)}$ $(1 \leqslant i \leqslant n)$ are canonical coordinates of a system with number α. Let us emphasize that n and H do not depend on α.

Let us introduce the unified phase space of dimension $2nN$ with canonical variables

$$(X, Y) = (x^{(1)}, y^{(1)}, \dots, x^{(N)}, y^{(N)})$$

and the Hamiltonian

$$\mathscr{H}_\varepsilon(X, Y) = \sum_{\alpha=1}^{N} H(x^{(\alpha)}, y^{(\alpha)}) + \varepsilon H_1(X, Y, \varepsilon), \tag{1.4}$$

where ε is a small parameter, which then will approach to zero. The system with the Hamiltonian (1.4) describes the dynamics of N weakly interacting subsystems with the Hamiltonians (1.3), and the function εH_1 denotes the interaction energy of subsystems.

The basic idea of derivation of Gibbs distribution is the assumption concerning the *ergodicity* of the system with the Hamiltonian (1.4) at $\varepsilon \neq 0$ on a level surface $\mathscr{H}_\varepsilon = NE$ [3]. Let f be an integrable function on a phase space of a system with n degrees of freedom. According to an indistinguishability principle, in statistical mechanics one considers only such functions of X and Y, which do not vary under permutations of groups of variables $x^{(\alpha)}$, $y^{(\alpha)}$. Let us assume that

$$F(X, Y) = \frac{1}{N} \sum_{\alpha} f(x^{(\alpha)}, y^{(\alpha)}). \tag{1.5}$$

Such functions are frequently called *summators*. Using ergodic hypothesis, we obtain for theaverage with respect to time (1.5) in the limit as $\varepsilon \to 0$ the formula

$$\langle F \rangle = \int f(x, y) \rho_N(x, y)\, dx\, dy\,.$$

The explicit expression for the density ρ_N can be found in [3]. With some additional suppositions [3] we can prove that $\rho_n \to \rho$ as $N \to \infty$ and for the average of function f along solutions of the system with the Hamiltonian (1.3) the formula

$$\langle f \rangle = \int f \rho\, dx\, dy$$

is valid.

On this way one has a series of fundamental difficulties. The main difficulty is the justification of the ergodic hypothesis. Only recently the ergodicity of some simplified models has been established [5]. Since the Gibbs distribution (1.1) does not depend on the form of an interaction energy H_1, F. A. Berezin [3] stated the idea of weakening of the ergodic hypothesis: it is enough to require ergodicity of the system with the Hamiltonian (1.4) for $\varepsilon \neq 0$ for set of functions H_1 everywhere dense. However, if the interaction energy H_1 has no singularities and surfaces of the energy level $\mathscr{H}_\varepsilon = NE$ are compact, the ergodic hypothesis (even in the weakened variant) isrefuted by the KAM-theory [6].

Example 1. Let us consider a system with the Hamiltonian, following [3]

$$\mathscr{H} = \frac{1}{2} \sum (x_\alpha^2 + \omega^2 y_\alpha^2) + \varepsilon V_4(x), \tag{1.6}$$

where $\omega = \text{const} \neq 0$, $V_4 \geqslant 0$ is a polynomial of the 4-th degree of coordinates $x_1, \dots, x_N$, $\varepsilon > 0$. Such systems play an essential role in the theory of heat capacities of rigid bodies [2]. The coefficients of non-negative polynomials of the 4-th degree form some set A in a finite-dimensional space of coefficients of

all polynomials of the 4-th degree from N variables. F. A. Berezin [3] has raised the following question: Is it correct, that for almost all points A the system with the Hamiltonian (1.6) is ergodic? The answer is negative. Indeed, let us consider polynomials of the form

$$V_4 = \sum_\alpha a_\alpha x_\alpha^4 + W_4(x)\,, \quad a_\alpha > 0\,,$$

and let the coefficients of the polynomial W_4 be small. If $W_4 = 0$, the system with the Hamiltonian (1.6) is integrated by a separation of variables. If we change to action-angle variables I_α, φ_α in a system with one degree of freedom

$$h_\alpha = \frac{(x^2 + \omega^2 y^2)}{2} + \varepsilon a_\alpha x^4\,,$$

then

$$\mu_\alpha = \frac{\partial h_\alpha}{\partial I_\alpha} > 0\,, \qquad \lambda_\alpha = \frac{\partial^2 h_\alpha}{\partial I_\alpha^2} > 0\,. \tag{1.7}$$

In the last inequality we essentially use the supposition, that $\varepsilon a_\alpha > 0$.

Let $H_0 = \sum h_\alpha(I_\alpha)$. If

$$\left\| \begin{matrix} \dfrac{\partial^2 H_0}{\partial I^2} & \dfrac{\partial H_0}{\partial I} \\ \dfrac{\partial H_0}{\partial I} & 0 \end{matrix} \right\| \neq 0\,, \tag{1.8}$$

then, according to the KAM-theory [6], the system with the Hamiltonian (1.6) is not ergodic on each positive energy level for small W_4 (when coefficients of W_4 are located in some small neighborhood of zero): the most part of this surface is foliated on N-dimensional invariant tori with conditional-periodic trajectories. In our case the determinant (1.8) is equal to

$$-\lambda_1 \ldots \lambda_n \left(\frac{a_1^2}{\lambda_1} + \ldots + \frac{a_n^2}{\lambda_n} \right),$$

what does not equal zero on account of (1.7).

It is still necessary to add that according to the above mentioned approach to the derivation of the Gibbs distribution (due to Darwin and Fouler (see [4])) the expression for the density of probability distribution (1.1) does not depend on the interaction of subsystems. While such an interaction is always present.

In this work we develop another approach to the justification of the formula for probability density due to classical works by Gibbs [1]. This approach will be based on the theory of integrability of Hamiltonian systems [7].

2. The main result

The statistical approach to the theory of dynamical systems assumes a refusal of consideration of separate trajectories. Instead, in the phase space of a system

$$\dot{x} = v(x) \tag{2.1}$$

we introduce the density of probability distribution $\rho(x,t) > 0$, explicitly depending on time in general case. Let D be any measurable area of the phase space, g^t be a phase flow of the system (2.1). This flow can be presented as a stationary flow of a fluid. Since the area $g^t(D)$ consists of the same moving phase points, it is natural to assume that the probability of detection of the system in the area $g^t(D)$ does not depend on t. Hence, this probability

$$\int\limits_{g^t(D)} \rho(x,t)\,dx$$

will be an integral invariant of the system (2.1). But then the density of probability distribution satisfies the Liouville equation:

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho v) = 0\,.$$

If $\operatorname{div} v = 0$, then ρ is a first integral of the system (2.1). This condition, obviously, holds for the Hamiltonian systems of differential equations. It is natural to consider stationary distributions for autonomous systems, when ρ does not depend on t explicitly. The detailed discussion of these problems can be found in [2, 4].

Locally, in a small neighbourhood of a nonsingular point the dynamical system (2.1) possesses a complete set of independent first integrals (in amount of $m-1$, where m is a dimension of the phase space). However, in a typical situation they can not be extended to single-valued integrals defined in the whole phase space. The density of probability distribution is a single-valued function on the phase space by definition. Generally Hamiltonian systems with compact level surfaces do not admit integrals independent of the Hamiltonian H, though they are not ergodic (on energy levels) [7]. This argument allows to state at once in some important cases, that

$$\rho = f(H)\,, \tag{2.2}$$

and to reduce the problem to determination of the form of function f.

However, the opposite point of view to the possibility of existence of additional integrals is widespread in physical literature (see, for example, [4], where the approach to justification of Gibbs distribution based on the formula (2.2) is called "speculative").

To show the possibilities of a new approach, let us consider a Hamiltonian system with n degrees of freedom. The Hamiltonian of this system has the form (1.4):

$$H = H_0 + \varepsilon H_1 + o(\varepsilon)\,, \quad H_0 = \sum h_i(x_i, y_i)\,, \quad H_1 = H_1(x_1, \dots, x_n, y_1, \dots, y_n)\,. \tag{2.3}$$

At $\varepsilon = 0$ the system splits into n independent subsystems with one degree of freedom. A system of connected pendula can be considered as an example.

Let us assume that in each one-dimensional system with a Hamiltonian h_i $(1 \leqslant i \leqslant n)$ we can introduce the canonical action-angle variables I_i, $\varphi_i \,(\mathrm{mod}\, 2\pi)$ [6]. For example, for a system with the Hamiltonian h_α from paragraph 1 such variables are defined in all phase space. In case of a pendulum the cylindrical phase space is divided by separatrices in three areas, in each area it is possible to introduce action-angle variables. In these variables

$$h_i = h_i(I_i)\,, \quad 1 \leqslant i \leqslant n\,. \tag{2.4}$$

Let us assume that the functions (2.4) are continuous and monotonically increasing. The naturality of this supposition follows from the definition of an action variable as a normalized area on a phase plane contained inside a phase curve $h_i = \mathrm{const}$. Then the variable I_i will be a single-valued function of energy h_i.

The above mentioned assumptions are not fulfilled in the case, when the potential energy of a system has some local minimums. However, these conditions have a technical character, and probably they can be essentially weakened.

Thus, in action-angle variables the Hamiltonian (2.3) has a form

$$H = \sum_{i=1}^{n} h_i(I_i) + \varepsilon H_1(I_1, \dots, I_n, \varphi_1, \dots, \varphi_n) + o(\varepsilon)\,. \tag{2.5}$$

It is 2π-periodic with respect to each angular variable $\varphi_1, \dots, \varphi_n$.

The density of probability distribution ρ for a system with the Hamiltonian (2.3) is a single-valued positive function of x, y, depending on parameter ε. Let us assume that ρ is a function from class C^2

(it possesses the second continuous derivative on a set of $2n+1$ variables x, y, ε). At small values of ε this function can be written as

$$\rho = \rho_0(x,y) + \varepsilon\rho_1(x,y) + o(\varepsilon)\,, \tag{2.6}$$

where ρ_0 and ρ_1 are functions from classes C^2 and C^1 respectively.

Now let ε tend to zero. Then ρ_0 will be a density of probability distribution for a system with the Hamiltonian

$$H_0 = h_1(x_1,y_1) + \ldots + h_n(x_n,y_n)\,.$$

This system with n degrees of freedom splits into n *independent* systems with one degree of freedom. The main independence property denotes that the motion of each of these subsystems is uniquely determinated by any of its initial states.

If we stick to the idea of statistical description of dynamical systems, it is necessary to introduce stationary densities of probability distribution

$$p_1(x_1,y_1),\ldots,p_n(x_n,y_n)$$

for each of one-dimensional systems. Taking into consideration the independence properties and using the probability product theorem, we obtain

$$\rho_0 = p_1\ldots p_n\,. \tag{2.7}$$

This equality is often called *Gibbs hypothesis on thermodynamic equilibrium* [2].

REMARK 1. One should not think that any separation of variables results in independent systems with one degree of freedom. Let us show this fact by a simple example :

$$2H_0 = y_2^2 + x_2^2\left[\frac{(y_1^2+x_1^2)}{2}\right]^2.$$

The variables x_2, y_2 perform simple harmonic oscillations, the frequency of which is equal to the energy of oscillations of the first subsystem (described by canonical coordinates x_1, y_1).

In the following, the Poincaré set $\mathbb{P}$ [7] plays an essential role. Let us decompose a disturbing function H_1 in a multiple Fourier series:

$$H_1 = \sum H^{(m)}(I_1,\ldots,I_n)\exp[i(m_1\varphi_1+\ldots+m_n\varphi_n)]\,,\quad m=(m_1,\ldots,m_n)\in\mathbb{Z}^n.$$

Let $\omega_i = \dfrac{dh_i}{dI_i}$ $(1\leqslant i\leqslant n)$ be the frequencies of a nonperturbed problem; and assume $\omega=(\omega_1,\ldots,\omega_n)$. By definition the set $\mathbb{P}$ consists of such points $I=(I_1,\ldots,I_n)\in\mathbb{R}^n$, for which there will be $n-1$ linearly independent integer vectors $\alpha,\alpha',\ldots\in\mathbb{Z}^n$, such that

1) $(\omega,\alpha)=(\omega,\alpha')=\ldots=0$;

2) $H^{(\alpha)}(I)\neq 0$, $H^{(\alpha')}(I)\neq 0,\ldots$.

In a typical situation the set $\mathbb{P}$ fills in the range of values $I\in\mathbb{R}^n$ [7] everywhere densely.

Our basic result is the following:

Theorem 1. *Let us assume, that systems with the Hamiltonians $h_1,\ldots,h_n$ are non-degenerate $\dfrac{d^2h_i}{dI_i^2}\neq 0$, the Poincaré set is everywhere dense and the condition* (2.7) *is fulfilled. Then*

$$\rho = ce^{-\beta H_0}(1+O(\varepsilon))\,, \tag{2.8}$$

where $c>0$, β are some constants.

The constant c is inessential: the result of averaging with respect to the measure (2.8)

$$\langle f\rangle = \frac{\int f\rho\,dxdy}{\int\rho\,dx\,dy}$$

does not depend on this constant. If $\varepsilon=0$ the formula (2.8) gives the Gibbs canonical distribution (1.1).

REMARK 2. We stress the fact, that (2.8) is valid for the fixed number of degrees of freedom $n \geqslant 2$. A. A. Vlasov [8] developed an approach to the derivation of Gibbs distribution, which would not use the analysis of interaction of subsystems at all and which is formally suitable for the case $n = 1$. This approach is based on the principle of "maximum statistical independence", which seems to be an artificial supposition.

3. Derivation of Gibbs distribution

The proof of Theorem 1 is based on application of the Poincaré method [9] in the form indicated in [7].

Setting $\varepsilon = 0$ according to (2.6) we obtain that ρ_0 is the first integral of a complete integrable Hamiltonian system with a Hamiltonian

$$H_0 = \sum_{k=1}^{n} h_k(I_k)\,.$$

Since nonperturbed system is non-degenerate, i. e.

$$\det \left\| \frac{\partial^2 H_0}{\partial I^2} \right\| = \prod_{k=1}^{n} \frac{d^2 h_k}{dI_k^2} \neq 0\,,$$

then the function ρ_0 expressed in action-angle variables I, $\varphi \bmod 2\pi$ depends only on $I_1, \ldots, I_n$ [7].

Furthermore, since ρ is the first integral of the canonical system of differential equations with a Hamiltonian H, their Poisson bracket is equal to zero: $\{\rho, H\} = 0$. Let us differentiate this equality with respect to ε and, then, let us assume $\varepsilon = 0$. Since ρ and H are supposed to be the functions of a class C^2 the differentiations with respect to phase variables and to the parameter ε are commutative. As a result we obtain the equality

$$\{\rho_0, H_1\} + \{\rho_1, H_0\} = 0\,,$$

from which, with the help of the Fourier method and by a known method [7], we can deduce that the functions $\rho_0(I_1, \ldots, I_n)$ and $H_o = \sum h_k(I_k)$ are dependent in all points of the Poincaré set $\mathbb{P}$. According to the supposition, this set is everywhere dense in a range of action variables I. Hence, the functions ρ_0 and H_0 are everywhere dependent by virtue of continuity.

The variables I_i may be presented as single-valued functions of h_i in accordance with the assumption made in Section 2 about properties of action-angle variables. Then $\rho_0 = \rho_0(h_1, \ldots, h_n)$ and $H_0 = \sum h_i$. Since these functions are dependent, ρ_0 is a smooth function of H_0.

Indeed, the condition of dependence of ρ_0 and H_0 gives relations

$$\frac{\partial \rho_0}{\partial h_i} = \frac{\partial \rho_0}{\partial h_j}\,, \tag{3.1}$$

which are valid for all values i, j. If we substitute $h_n = H_0 - h_1 - \ldots - h_{n-1}$ in the expression for ρ_0, we shall obtain

$$\rho_0 = f(H_0, h_1, \ldots, h_{n-1}) = \rho_0 \left(h_1, \ldots, h_{n-1}, H_0 - \sum_{k=1}^{n-1} h_k \right)\,.$$

However, this function does not actually depend on $h_1, \ldots, h_{n-1}$, since

$$\frac{\partial f}{\partial h_i} = \frac{\partial \rho_0}{\partial h_i} - \frac{\partial \rho_0}{\partial h_n} = 0\,, \quad i < n$$

according to (3.1).

The probability densities $p_1, \ldots, p_n$ are the integrals of one-dimensional systems with Hamiltonians $h_1, \ldots, h_n$. Hence, in the action-angle variables, p_i are smooth functions only of I_i. But in this case p_i is a single-valued differentiable function of the energy h_i.

Thus, the equality (2.7) can be presented in the following form :

$$\rho_0(h_1 + \ldots + h_n) = p_1(h_1) \ldots p_n(h_n)\,.$$

Consecutively differentiating this relation with respect to $h_1, \ldots, h_n$ and using the positiveness of functions $p_1, \ldots, p_n$, we obtain equalities

$$\frac{p_1'}{p_1} = \ldots = \frac{p_n'}{p_n} = -\beta\,,$$

where β is some constant. Hence,

$$p_i = c_i e^{-\beta h_i}\,, \qquad c_i = \text{const} > 0\,, \tag{3.2}$$

and consequently

$$\rho_0 = c e^{-\beta H_0}\,, \qquad c = c_1 \ldots c_n > 0\,.$$

The theorem is proved.

REMARK 3. As we see from (3.2), the constant β is one and the same for all subsystems. It means that the weakly interacting subsystems are in the thermodynamic equilibrium (and in the limit as $\varepsilon \to 0$), since their temperatures $T = \dfrac{1}{\beta k}$ are identical. Thus, when $\varepsilon \to 0$, the statistical independence of subsystems is equivalent to their thermodynamic equilibrium. This is the physical sense of the Gibbs hypothesis.

4. Analytical case

In the applications, the Hamiltonian (3.2) is an analytical function of phase variables and the parameter ε. In this case it is also natural to consider the probability density (2.6) as an analytical function with respect to x, y, ε.

The condition of everywhere-density of the Poincaré set can be weakened: it is enough to require, that $\mathbb{P}$ would be a key set for a class of analytical functions. It means the following: if the analytical function $f(I)$ is equal to zero in the points of $\mathbb{P}$, then $f \equiv 0$. The examples of nondense key sets may be found in [7]. In particular, if the analytical functions are dependent in the points $\mathbb{P}$, they are everywhere dependent.

Theorem 2. *Let us assume, that the systems with Hamiltonians $h_1, \ldots, h_n$ are non-degenerate, the Poincaré set is a key set for the class of analytical functions and the equality* (2.7) *is performed. Then the analytical density of probability distribution for the system with the Hamiltonian* (2.3) *has the form*

$$\rho = c e^{-\beta H}[1 + \varepsilon g(H, \varepsilon)]\,, \tag{4.1}$$

where $c > 0$, $\beta \neq 0$ are some constants, g is an analytical function of the energy H and the parameter ε.

The function g can be represented as a power series in terms of ε with coefficients depending on the energy H only. The summand εg in (4.1) is completely analogous to the Gram–Charlier series in the theory of distribution of random variables which are unessentially different from the normal distributed ones (see, for example, [10]).

Proof.

Let us prove Theorem 2. Expand the probability density in the power series of ε:

$$\rho = \rho_0 + \varepsilon\rho_1 + \varepsilon^2\rho_2 + \dots .$$

On account of non-degeneracy of the unperturbed system, ρ_0 is an analytical function of action variables I only. Since ρ_0 and H_0 are dependent at points $I \in \mathbb{P}$, and $\mathbb{P}$ is the key set, ρ_0 and H_0 are dependent everywhere. Therefore, taking into consideration the Gibbs hypothesis (2.7),

$$\rho_0 = ce^{-\beta H_0}\,; \quad c, \beta = \text{const},$$

(see Section 3). Since $\rho_0 > 0$, we have $c > 0$. The constant β is not equal to zero, otherwise ρ_0 is not the density of probabilistic measure (the volume of the whole phase space is infinite).

Further, the analytical function

$$\frac{\rho}{ce^{-\beta H}}$$

is an integral of Hamilton equations with the Hamiltonian (2.7). Let us expand this function in power series of ε: $1 + \varepsilon G_0 + \varepsilon^2 G_1 + \dots$. It is obvious that the series

$$G_0 + \varepsilon G_1 + \dots \tag{4.2}$$

is an integral of the same system. With the help of the method used in Section 3 one can prove that G_0 is an analytical function of H_0: $G_0 = g_0(H_0)$. It is obvious that the power series

$$\frac{[G_0 + \varepsilon G_1 + \dots - g_0(H)]}{\varepsilon} = F_0 + \varepsilon F_1 + \dots$$

is again a first integral. Thus, F_0 is an analytical function of H_0: $F_0 = g_1(H_0)$. Extending infinitely this procedure, we obtain that the series (4.2) has actually the form:

$$g_0(H) + \varepsilon g_1(H) + \dots .$$

Denoting this function by $g(H, \varepsilon)$, we obtain the desired formula (4.1). ■

REMARK 4. Let us introduce $K(H, \varepsilon)$ by setting

$$\rho = ce^{-\beta K}, \tag{4.3}$$

where the density ρ is given by (4.1). The function K can be expanded in power series $K_0 + \varepsilon K_1 + \dots$, where

$$K_0 = H_0\,, \quad K_1 = H_1 - \frac{g_0(H_0)}{\beta}, \dots .$$

Hamilton equations with the Hamiltonians H and K possess the same trajectories, however, times of motion along these trajectories are different. The formula (4.3) implies the Gibbs canonical distribution for a slightly changed Hamiltonian system.

5. Application to the system of weakly connected pendula

Let us consider n identical mathematical pendula of mass m and length l, consecutively connected with each other by elastic springs with small rigidity $\varkappa$. For the simplicity we assume that the fixed points of pendula coincide. This system with n degrees of freedom is described by canonical differential equations with the Hamiltonian $H_0 + \varepsilon H_1$, where

$$H_0 = \sum_{i=1}^{n} \frac{y_i^2}{2ml^2} - mgl\cos x_i\,, \qquad H_1 = \sum_{i=1}^{n-1} \cos(x_i - x_{i+1})\,,$$

$\varepsilon = -\frac{\varkappa l^2}{4}$ is a small parameter. The transition to angle-action variables is carried out for the pendulum with the help of elliptic functions (see, for example, [7]). It is possible to show that the Fourier series of perturbation function with respect to angle variables $\varphi_1, \ldots, \varphi_n \bmod 2\pi$ has the form:

$$H_1 = \sum_{m_1,m_2} h_{m_1,m_2}(I_1) e^{2i(m_1\varphi_1 + m_2\varphi_2)} + \ldots + \sum_{m_{n-1},m_n} h_{m_{n-1},m_n}(I_n) e^{2i(m_{n-1}\varphi_{n-1} + m_n\varphi_n)}\,.$$

The summation is taken over all integer $m_1, \ldots, m_n$ from $-\infty$ to $+\infty$. The coefficients in this expansion can be expressed explicitly with the help of known expansions of elliptic functions sn^2, cn^2 and $sncn$ in Fourier series [11]. All of them are not equal to zero.

The Poincaré set $\mathbb{P}$ is defined in this problem as the set of points $I = (I_1, \ldots, I_n)$, satisfying $n-1$ equations

$$m_1\omega_1(I_1) + m_2\omega_2(I_2) = \ldots = m_{n-1}\omega_{n-1}(I_{n-1}) + m_n\omega_n(I_n) = 0\,,$$

where either $m_1 m_2 \ldots m_{n-1} \neq 0$ or $m_2 m_3 \ldots m_n \neq 0$. If one of the two latter conditions is fulfilled, the vectors $(m_1, m_2, 0, \ldots, 0)$, $(0, m_2, m_3, 0, \ldots, 0)$, $\ldots$, $(0, 0, \ldots, m_{n-1}, m_n)$ are linearly independent. It is possible to show that the set $\mathbb{P}$, which consists of infinitely many curves, fills in the domain of definition of action variables $\{I_1 \geqslant 0, \ldots, I_n \geqslant 0\}$ everywhere densely.

Thus, the statements of Theorems 1 and 2 are valid for the chain of connected pendula. If one of the springs is taken away, the system splits into two disconnected chains, the Hamiltonians of which are the first integrals of the total system. In this case the density of probability distribution is not the function of the total energy of the system only and thus is not subjected to the Gibbs distribution.

6. Thermodynamics of mechanical systems

Let us consider a Hamiltonian system with the Hamiltonian H, where the density of probability distribution is defined by the Gibbs formula (1.1). According to theorem 1, it can be a system with n degrees of freedom, composed of independent one-dimensional subsystems, or one of these subsystems. We shall show, after Gibbs [1], that this mechanical system can be naturally connected with some thermodynamic system.

Let us assume that the Hamiltonian H depends not only on canonical variables x, y, but also on several parameters $\lambda_1, \ldots, \lambda_m$. One can take, for example, the length of the pendulum as such a parameter. The parameters λ can be considered as generalized coordinates of some system with $n+m$ degrees of freedom and the constancy of λ as application of holonomic constraints. Thus, let $H_*(x, y, \lambda, \mu)$ be the Hamiltonian of a system with $n+m$ degrees of freedom, $\mu_1, \ldots, \mu_m$ be canonical momenta conjugated with additional coordinates $\lambda_1, \ldots, \lambda_m$. The dynamics of the extended system is described by the canonical equations

$$\dot{x} = \frac{\partial H_*}{\partial y}\,, \qquad \dot{y} = -\frac{\partial H_*}{\partial x}\,, \qquad \dot{\lambda} = \frac{\partial H_*}{\partial \mu}\,, \qquad \dot{\mu} = -\frac{\partial H_*}{\partial \lambda}\,. \tag{6.1}$$

Let us impose m independent relations $\lambda_1, \ldots, \lambda_m = \text{const}$ on this system. Therefore, $\dot{\lambda}_i = 0$, and from the equations

$$\frac{\partial H_*}{\partial \mu_1} = \ldots = \frac{\partial H_*}{\partial \mu_m} = 0 \tag{6.2}$$

one can derive momenta μ as functions of x, y and constant parameters λ. The sufficient condition of solvability of the equations (6.2) with respect to μ is reduced to the inequality

$$\det \left\| \frac{\partial^2 H_*}{\partial \mu_i \partial \mu_j} \right\| \neq 0\,.$$

It is fulfilled automatically if H_* is a positively defined quadratic form of $n+m$ momenta y, μ.

Substituting the obtained expressions for μ in the last set of equations (6.1), we obtain additional relations on canonical variables x, y, which, of course, are not fulfilled in general case. Therefore, it is necessary to introduce additional forces, the constraint reactions $R_1, \ldots, R_m$, and replace the latter equation of (6.1) by

$$\dot{\mu} = -\frac{\partial H_*}{\partial \lambda} + R\,. \tag{6.3}$$

Let $\mu = \mu(x, y, \lambda)$ be a solution of the algebraic system (6.2). We assume that

$$H(x, y, \lambda) = H_*(x, y, \lambda, \mu(x, y, \lambda)).$$

On account of (6.2),

$$\frac{\partial H}{\partial x} = \frac{\partial H_*}{\partial x}\,, \qquad \frac{\partial H}{\partial y} = \frac{\partial H_*}{\partial y}\,, \qquad \frac{\partial H}{\partial \lambda} = \frac{\partial H_*}{\partial \lambda}\,.$$

Consequently, for constant values of λ the variables x, y change according to Hamilton equations with the Hamiltonian H, and the equation (6.3) can be replaced by

$$\dot{\mu} = -\frac{\partial H}{\partial \lambda} + R\,. \tag{6.4}$$

Let $x(t, x_0, y_0)$, $y(t, x_0, y_0)$ be solutions of canonical equations with the Hamiltonian H. We assume that for every such solution $\mu(t)/t \to 0$ as $t \to +\infty$. Then the time-average of $\dot{\mu}$ is equal to zero. This assumption is automatically fulfilled if the configuration space $\{x\}$ is compact: on account of existence of energy integral the function $\mu(t)$ is bounded.

At first let us average both parts of the equality (6.4) with respect to time and then with respect to the measure $\rho(x_0, y_0)dx_0dy_0$, where ρ is given by (1.1). According to the Birkhoff–Khinchin ergodic theorem [12] the obtained relation is equivalent to the following one:

$$\langle R \rangle = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle\,. \tag{6.5}$$

Here $\langle\ \rangle$ is the mean with respect to the Gibbs measure (1.1).

REMARK 5. Usually [3, 4] the relation (6.5) is derived from the simplified relation of (6.4), which lacks the derivative $\dot{\mu}$.

The relation (1.2) defines the "internal" energy E as a function of parameters $\lambda_1, \ldots, \lambda_m$ and β (recall that $\beta^{-1} = kT$). Let us set $\Lambda = -\langle R \rangle$, i.e., the phase mean values of the above introduced constraint reactions (with the opposite sign). The relations

$$\Lambda_i = f_i(\lambda_1, \ldots, \lambda_m, \beta)\,, \quad 1 \leqslant i \leqslant m \tag{6.6}$$

are usually called in thermodynamics the equations of state. Assignment of functions E and Λ_i is included in the definition of thermodynamic system. However, these functions can not be arbitrary, since the first and the second principles of thermodynamics must be fulfilled.

Let us introduce the statistical integral

$$Z(\lambda, \beta) = \int e^{-\beta H}\, dx\, dy\,.$$

One can verify the validity of the equalities [3, 4]

$$\Lambda_i = \frac{1}{\beta}\frac{\partial \ln Z}{\partial \lambda_i}, \quad (1 \leqslant i \leqslant m)\,, \qquad E = -\frac{\partial \ln Z}{\partial \beta}\,. \tag{6.7}$$

In thermodynamics the main role plays the differential 1-form of heat gain

$$\omega = dE + \sum \Lambda_i \, d\lambda_i \, .$$

Motivations for this definition can be found in [2, 4]. According to the first equality of (6.7) the form ω is the exact differential for fixed values of β (or absolute temperature T). This is the first principle of thermodynamics. Then, taking into account (6.7) we obtain

$$\beta\omega = \beta \, dE + \sum \Lambda_i \, d\lambda_i = d(\beta E) - E \, d\beta + \sum \Lambda_i \, d\lambda_i = d(\beta E + \ln Z) \, .$$

Thus, the form of heat gain possesses the integrating factor $\beta = 1/(kT)$. This is the second principle of thermodynamics. The function $S = \beta E + \ln Z$ is the entropy of thermodynamic system.

Finally, let us give an illustrative example. We consider a motion of a point of mass m, attached to the end of unstretchable thread of length l. Let x be the angle of rotation of the thread, y be the conjugate canonical momentum. If active forces are not applied to the point, its dynamics is described by canonical equations with the Hamiltonian

$$H = \frac{y^2}{2ml^2} \, .$$

Let us take the length of the thread l as the parameter λ. The statistical integral is equal to

$$Z = (2\pi)^{3/2} m^{1/2} l \beta^{-1/2} .$$

Let p be a force, corresponding to the parameter l (the thread tension). Then, according to (6.7) the equation of state (6.6) has the form $p = 1/(\beta l)$ or $pl = kT$. It is similar to the ideal gas law. The second equation (6.7) gives the relation for the internal energy $E = 1/(2\beta)$ or $E = kT/2$. From these relations we obtain the formula $p = 2E/l$, which, however, was valid before the application of averaging procedure.

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