

## THE CONNECTION BETWEEN THERMODYNAMIC ENTROPY AND PROBABILITY\*

V.L. BERDICHEVSKII

Ergodic Hamiltonian systems with an arbitrary number of degrees of freedom  $n$  are considered. A relation is derived connecting the distribution function of the system characteristics with the entropy. It is shown that as  $n \rightarrow \infty$  it reduces to Einstein's formula /1/. A variational principle for the distribution function, which reduces to the maximum-uncertainty principle as  $n \rightarrow \infty$ , is derived. The principle of maximum entropy for Hamiltonian systems is formulated.

1. **The thermodynamics of Hamiltonian systems.** According to the Boltzmann program of the basis of thermodynamics, thermodynamic relations can be obtained by averaging the Hamilton equations. The first non-trivial problem which then arises is the problem of interpreting entropy in terms of mechanics. Boltzmann's answer was the following equation:

$$S = k \ln W \quad (1.1)$$

where  $k$  is a constant which depends on the choice of the units of measurements, and  $W$  is the number of microstates corresponding to a specified macrostate. Formula (1.1) is of considerable heuristic importance, but it is not entirely complete, since the meaning of the number of microstates for a Hamiltonian system is somewhat obscure. A final answer was obtained by Gibbs /2/ and was subsequently investigated from new points of view by Hertz /3/ (the results obtained by Gibbs and Hertz are formulated below in modern terms).

Einstein /1/ proposed the following interpretation of Boltzmann's formula (1.1). Suppose  $z_1, \dots, z_k$  are parameters describing the thermodynamic system, and  $S(z_1, \dots, z_k)$  is the entropy of the system. In a state of thermodynamic equilibrium the system parameters fluctuate and have a certain density of the distribution function  $f(z_1, \dots, z_k)$ . According to /1/ we have

$$f(z_1, \dots, z_k) = \text{const} \cdot \exp S(z_1, \dots, z_k) \quad (1.2)$$

The constant in front of the exponent is determined from the conditions for normalizing the distribution function. The discussions in /1, 4/, which indicate the correctness of Eq. (1.2), relate to system with a large number of degrees of freedom  $n$  and parameters which only differ slightly from the mean values. Below, for ergodic Hamiltonian systems, we obtain an exact formula which holds for any  $n$  and fluctuations of arbitrary amplitude. Einstein's formula (1.2) is obtained from the accurate one in the limit as  $n \rightarrow \infty$ .

The problem considered is intimately related to the reappraisal of the fundamentals of statistical mechanics which is going on at the moment. Earlier it was generally recognised that the laws of thermodynamics and statistical mechanics are due to the large number of degrees of freedom of the mechanical system performing a complex stochastic motion. The problem was that essentially large  $n$  or stochasticity did not occur, since there were no physically interesting examples of systems with stochastic behaviour and finite  $n$  (with the exception, of course, of geodesic flow in manifolds of negative curvature, which are outside the field of view of physicists). The discovery of such systems (see /5-9/) made this question extremely important. The assertions formulated below show that ergodic Hamiltonian systems with any  $n$  (including small values of  $n$ ) correspond to a large extent to the representations of both equilibrium thermodynamics and statistical mechanics. In this case some assertions (Einstein's formula and the principle of maximum uncertainty) require some modification, while in others, of several formulations which merge in the limit as  $n \rightarrow \infty$ , we must choose one universal one which holds for all  $n$  (these include the definition of entropy and the second law of thermodynamics).

We will start with a description of the necessary facts from the theory of Hamiltonian systems.

*Ergodic Hamiltonian systems.* We will consider a mechanical system with generalized coordinates  $q^i (i=1, \dots, n)$  and generalized momenta  $p_i$ . Suppose  $H(p, q, y)$  is the Hamilton function and  $y = (y^1, \dots, y^r)$  are external parameters, the change in which corresponds to the change in the external conditions. The system is described by Hamilton's equations

\*Prikl. Matem. Mekhan., 52, 6, 947-957, 1988

$$\frac{dp_i}{dt} = -\frac{\partial H(p, q, y)}{\partial q^i}, \quad \frac{dq^i}{dt} = \frac{\partial H(p, q, y)}{\partial p_i} \quad (1.3)$$

We will assume initially that the values of the parameters  $y$  are fixed. Then Eqs. (1.3) have a first integral  $H(x, y) = \text{const}$  (we henceforth denote by  $x$  the points of phase space of the variables  $p, q$ ) and each trajectory starting from the surface of the energy level  $H(x, y) = \text{const}$ , lies completely on it. The surfaces of the level are assumed to be compact, and bound a finite volume.

Suppose  $\Sigma$  is a certain surface of the energy level. Each point  $x$  on  $\Sigma$  in a time  $t$  travels along a trajectory of system (1.3) to a certain point  $x_t$ , and correspondingly each region  $A$  on  $\Sigma$  transfers to a certain region  $A_t$ . The Euclidean areas of the regions  $A, A_t$ , generally speaking, are different, but they can be established using Liouville's theorem (see, for example, /10/, the quantity  $\int_A |\nabla_x H|^{-1} d\sigma$  is preserved, where  $d\sigma$  is the Euclidean of the element of area, while the modulus of the vector  $\nabla_x H = (\partial H / \partial x^i)$  is also understood in the Euclidean sense. Hence, if we introduce a measure of the region  $A$ , normalized to unity, by means of the formula

$$\mu(A) = \frac{\int_A |\nabla_x H|^{-1} d\sigma}{\int_{\Sigma} |\nabla_x H|^{-1} d\sigma} \quad (1.4)$$

it will be invariant under shifts along the trajectories of system (1.3).

The Hamiltonian of the system is called ergodic if there are no other invariant measures in it. The condition of ergodicity is essentially the most compact formulation of the fact that (almost) every trajectory of the system winds round the whole isoenergetic surface and no room can be found on any part of it.

For ergodic Hamiltonian systems the Birkhoff-Khinchin theorem holds (see /7, 10/): the time-average and the measure-average are identical, i.e. for any function  $\varphi(x)$  and (almost) any trajectory

$$\lim_{\theta \rightarrow \infty} \frac{1}{\theta} \int_0^\theta \varphi(x_t) dt = \int_{\Sigma} \varphi(x) |\nabla_x H|^{-1} d\sigma / \int_{\Sigma} |\nabla_x H|^{-1} d\sigma \quad (1.5)$$

As a rule, the proof of the ergodicity of specific mechanical systems encountered in mechanics and physics is an extremely complex mathematical problem (the results obtained up to the present time are collected in /7/), and hence, we can take as the basis for constructing statistical mechanics, instead of other hypotheses of a physical nature, which one is obliged to do all the same, the assumption that the system considered is ergodic, bearing in mind the consequences to which this leads.

*Entropy.* The term "entropy" is used in science in several different meanings (we may mention the corresponding ideas in phenomenological thermodynamics, information theory, the theory of dynamic systems and topology). Our aim is to determine the entropy of a Hamiltonian system so that it most accurately corresponds to the entropy of phenomenological thermodynamics. To do this we will consider an example - an adiabatically insulated vessel with a gas. We will take the following Hamiltonian system as the microscopic model of the gas: a large number of absolutely solid spheres colliding absolutely elastically with one another and with the walls of the vessel. The spheres model and molecules of a gas and the elastic collisions with the walls correspond to the assumption that the system is adiabatically insulated. We will slowly change the volume of the vessel  $V$ . Then work is done on the gas and its energy  $E$  is changed. In accordance with the laws of thermodynamics a function  $S(E, V)$  exists called the entropy which remains constant during this process.

In the Hamiltonian system a slow change in the parameters  $y$ , which occurs in the Hamilton function corresponds to the change in the volume, while the function of the energy of the system  $E$  and the parameters  $y$ , which does not change when there is a slow change in  $y$ , corresponds to the entropy. In the theory of Hamiltonian systems such functions are called adiabatic invariants. In ergodic Hamiltonian systems there is an adiabatic invariant, namely, the volume  $\Gamma$  of the region of phase space bounded by the surface  $H(x, y) = E$

$$\Gamma(E, y) = \int_{H(x, y) \leq E} d^{2n}x \quad (1.6)$$

This assertion is in fact contained in Gibbs' results /2/ and was established once again and first used as the fundamental initial assertion of Hertz's statistical mechanics /3, 11/ (see also /12/). An accurate mathematical formulation and proof can be derived from Anosov's

averaging theorem /13/, and is given independently in /14/. All the remaining adiabatic invariants are functions of  $\Gamma$  (this assertion was announced in /14/).

Thus the entropy of the Hamiltonian system is a certain function of  $\Gamma$ ; its form is established below.

*Temperature.* We will calculate the mean value along the trajectory of the system (denoted by the symbol  $\langle \cdot \rangle$ ) of the quantity  $x_i \partial H / \partial x_j$  (the subscripts  $i$  and  $j$  on  $x$  take values of  $1, \dots, 2n$ ). According to (1.5) we have

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \int_{\Sigma} x_i \frac{\partial H}{\partial x_j} |\nabla_x H|^{-1} d\sigma / \int_{\Sigma} |\nabla_x H|^{-1} d\sigma \quad (1.7)$$

$(\partial H / \partial x_j) |\nabla_x H|^{-1}$  are the components of the unit vector of the external normal to  $\Sigma$ , and hence we can change in the numerator in (1.7) from integration over the surface to integration of the volume using Stokes' theorem. The integral over the volume is equal to  $\Gamma \delta_{ij}$ . We can establish the following relationship for the denominator in (1.7):

$$\frac{\partial \Gamma(E, y)}{\partial E} = \int_{\Sigma} |\nabla_x H|^{-1} d\sigma \quad (1.8)$$

Hence, we obtain for the average value of  $\langle x_i \partial H / \partial x_j \rangle$

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \frac{\Gamma}{\partial \Gamma / \partial E} \delta_{ij} \quad (1.9)$$

Eq.(1.9) contains much important information. Henceforth we will only require one of its corollaries, which is obtained if we substitute as  $x_i$  in (1.9) the momenta

$$\left\langle p_1 \frac{\partial H}{\partial p_1} \right\rangle = \dots = \left\langle p_n \frac{\partial H}{\partial p_n} \right\rangle = \frac{\Gamma}{\partial \Gamma / \partial E} \quad (1.10)$$

For Hamiltonian functions that are quadratic in the momenta the quantity  $\langle p_1 \partial H / \partial p_1 \rangle$  has the meaning of twice the kinetic energy taken over the first degree of freedom, and Eq.(1.10) denotes that in ergodic Hamiltonian system the mean kinetic energy taken over each degree of freedom is the same. This quantity, by definition, is called the temperature of the system  $T$ .

A comparison of the equation  $T = \Gamma (\partial \Gamma / \partial E)^{-1}$  and the thermodynamic relation

$$1/T = \partial S(E, y) / \partial E \quad (1.11)$$

shows that Eq.(1.11) will hold for Hamiltonian systems if the entropy of the system is given by the equation

$$S = \ln \Gamma(E, y) + \text{const} \quad (1.12)$$

In text books on statistical mechanics another definition is usually given of the entropy:  $S = \ln(\Delta E \partial \Gamma / \partial E)$ , where  $\Delta E$  is a certain energy range defined in a special way. For "proper" systems as  $n \rightarrow \infty$  this definition agrees with (1.12), but they are different for finite values of  $n$ . Statistical mechanics, based on Eq.(1.12), was described by Hertz in the text book /11/, but, unfortunately, this had no influence on the modern form of statistical mechanics. Of the scores of courses on statistical mechanics known to the author, formula (1.12) is only given in /15/ (without any mention of the adiabatic invariance of  $\Gamma$ ), while in /16/ it is discussed in a single problem. On the other hand, relations (1.7)-(1.10) can be found in practically all courses, often with facts which only hold for large  $n$ .

**2: The distribution function of the parameters.** Consider any characteristic  $\Phi$  of the system, which is a smooth function of the generalized coordinates and momenta:  $\Phi = \Phi(x)$ . The probability that the values of  $\Phi$  lie in the range  $(z, z + dz)$ , which is equal to the fraction of the time which the function  $\Phi(x_t)$  spends in this interval, is equal to the integral (1.4) in which  $A$  must be understood as part of the surface  $\Sigma$ , defined by the inequalities  $z \leq \Phi(x) \leq z + dz$ . This fact can be derived from the Birkhoff-Khinchin theorem (1.5) (see, for example, /10/). We will denote by  $\Gamma(E, z, y)$  the volume of the region in phase space bounded by the surfaces  $H(x, y) \leq E$ ,  $\Phi(x) \leq z$  (we assume that the hypersurfaces  $\Phi(x) = z$  are transversal to the surface of the energy levels  $H(x, y) = E$ ), and we let  $f(z)$  be the distribution function density of the quantity  $\Phi$ .

The following formula holds:

$$f(z) = \frac{\partial^2 \Gamma(E, z, y)}{\partial E \partial z} / \frac{\partial \Gamma(E, y)}{\partial E} \quad (2.1)$$

The function  $f(z)$  depends, of course, on  $E$  and  $y$ , but this is not indicated in the notation.

Before proving (2.1) we will make a few preliminary observations. When  $x$  varies in the range  $H(x, y) \leq E$ , the value of  $\Phi(x)$  changes in the range  $[z^-, z^+]$ ,  $z^- = \min_{x: H(x, y) \leq E} \Phi(x)$ ,  $z^+ = \max_{x: H(x, y) \leq E} \Phi(x)$ . Hence, the function  $\Gamma(E, z, y)$  is equal to zero when  $z \leq z^-$ . When  $z \geq z^+$  the limitation  $\Phi(x) \leq z$  holds for all  $x$  inside the isoenergetic surface, and hence the function  $\Gamma(E, z, y)$  is constant with respect to  $z$  and is equal to  $\Gamma(E, y)$ . Consequently,  $f(z) = 0$  when  $z \leq z^-$  or  $z \geq z^+$ , as it should be. Further, integrating (2.1) with respect to  $z$ , it can be shown that the following normalization condition is satisfied:

$$\int_{-\infty}^{+\infty} f(z) dz = \int_{z^-}^{z^+} \frac{\partial^2 \Gamma(E, z, y)}{\partial E \partial z} dz / \frac{\partial \Gamma(E, y)}{\partial E} = 1 \quad (2.2)$$

We will now prove (2.1). Consider a volume of the region enclosed between the surfaces  $H(x, y) = E$ ,  $H(x, y) = E + \Delta E$ ,  $\Phi(x) = z$ ,  $\Phi(x) = z + \Delta z$ . It is obviously equal to  $\Gamma(E + \Delta E, z + \Delta z, y) - \Gamma(E, z + \Delta z, y) - (\Gamma(E + \Delta E, z, y) - \Gamma(E, z, y)) = \Delta E \Delta z \partial^2 \Gamma / \partial E \partial z$ . On the other hand, this same volume is equal to  $f(z) \Delta z \Delta E \partial \Gamma(E, y) / \partial E$ . Equating both quantities we obtain (2.1).

If there are several independent characteristics of the system  $\Phi_1(x), \dots, \Phi_k(x)$ , then, denoting the volume of the region defined by the limitations  $H(x, y) \leq E$ ,  $\Phi_1(x) \leq z_1, \dots, \Phi_k(x) \leq z_k$  by  $\Gamma(E, z_1, \dots, z_k, y)$ , we arrive in exactly the same way at the following formula for the distribution function density of the quantities  $\Phi_1, \dots, \Phi_k$ :

$$f(z_1, \dots, z_k) = \frac{\partial^{k+1} \Gamma(E, z_1, \dots, z_k, y)}{\partial E \partial z_1 \dots \partial z_k} / \frac{\partial \Gamma(E, y)}{\partial E} \quad (2.3)$$

A comparison of the accurate Eqs. (1.12) and (2.3) suggests the following program for proving Einstein's formula. The numerator in (2.3) can be regarded as the volume of a  $[2n - (k + 1)]$ -dimensional region, defined by the constraints  $H = E$ ,  $\Phi_1 = z_1, \dots, \Phi_k = z_k$ . If we succeed in constructing an auxiliary Hamiltonian system containing ergodic motion in this region, the volume must be proportional to  $\exp S$ , where  $S$  is the entropy of the auxiliary system, and we arrive at formula (1.2). In fact, as will be shown below, the quantity  $\partial^k \Gamma(E, z, y) / \partial z_1 \dots \partial z_k$  will be an adiabatic invariant, and hence

$$\frac{\partial^k \Gamma(E, z, y)}{\partial z_1 \dots \partial z_k} = \exp S(E, z, y) \quad (2.4)$$

and the correct formula has the form

$$f(z) = \frac{1}{\partial \Gamma(E, y) / \partial E} \frac{\partial}{\partial E} \exp(S(E, z, y)) \quad (2.5)$$

It can also be rewritten in a form which makes its connection with Einstein's formula obvious

$$f(z) = (\partial \Gamma(E, y) / \partial E)^{-1} \exp S(E, z, y) + \ln S_E \quad (2.6)$$

where  $S_E \equiv \partial S(E, z, y) / \partial E$ . For typical Hamiltonian systems of statistical mechanics, as  $n \rightarrow \infty$  the entropy increases in proportion to  $n$ , while the inverse temperature  $S_E$  is limited, and hence the value of  $\ln S_E$  can be neglected compared with  $S$  and (2.6) reduces to Einstein's formula (1.2).

We will now prove Eq. (2.5).

3. The entropy of Hamiltonian systems with bounds. Consider a system with a Hamiltonian function  $H(x, y)$  and bounds  $\Phi_1(x) = z_1, \dots, \Phi_k(x) = z_k$ . If  $\Phi_\alpha(x)$  ( $\alpha = 1, 2, \dots, k$ ) depends only on the coordinates, these are the usual kinematic limitations. If  $\Phi_\alpha(x)$  also depend on the momenta, the corresponding limitations, generally speaking, are non-holonomic. The theory of such systems is investigated in vacuum mechanics (see /17/). The trajectories of the system are found by solving the following system of equations (with respect to repeated indices of summation)

$$\frac{dp_i}{dt} = - \frac{\partial H}{\partial q^i} - \lambda^\alpha \frac{\partial \Phi_\alpha}{\partial q^i}, \quad \frac{dq^i}{dt} = \frac{\partial H}{\partial p_i} + \lambda^\alpha \frac{\partial \Phi_\alpha}{\partial p_i} \quad (3.1)$$

The Lagrange multipliers  $\lambda^\alpha$  are the required functions of time defined from the conditions  $d\Phi_\alpha/dt = 0$ . These conditions, using (3.1), can be rewritten in the form

$$\frac{d\Phi_\alpha}{dt} = [\Phi_\alpha, H] + \lambda^\beta [\Phi_\alpha, \Phi_\beta] = 0 \quad (3.2)$$

where  $[, ]$  are Poisson brackets. Eqs.(3.2) can be regarded as a system of linear equations in  $\lambda^\alpha$ . We will assume that the determinant of system (3.2) is non-zero:

$$\det \|\Phi_\alpha, \Phi_\beta\| \neq 0 \quad (3.3)$$

Then  $\lambda^\alpha$  in view of (3.2), will be universal functions of the coordinates of phase space, and system (3.1) becomes the usual autonomous system of differential equations.

Condition (3.3) imposes considerable limitations on the choice of the system parameters. In particular, their number  $k$  must be even, since the matrix with elements  $[\Phi_\alpha, \Phi_\beta]$  is skew-symmetric and its determinant is identically equal to zero for odd  $k$ .

If  $\lambda^\alpha$  are found from (3.2), the functions  $\Phi_\alpha$  are the first integrals of system (3.1). Moreover, there is also an energy integral, since

$$dH/dt = \lambda^\alpha [H, \Phi_\alpha] \quad (3.4)$$

and, convoluting (3.2) with  $\lambda^\alpha$  and taking into account the fact that in view of the antisymmetry of  $[\Phi_\alpha, \Phi_\beta]$  their convolution with a symmetrical object  $\lambda^\alpha \lambda^\beta$  is zero, we obtain that the right-hand side of (3.4) is also equal to zero.

We will assume that Eqs.(3.1) do not have other first integrals apart from  $H$  and  $\Phi_\alpha$ , and the motion in layers  $H = \text{const}$ ,  $\Phi_\alpha = \text{const}$  is ergodic. We will also assume that the phase volume does not change for motion along the trajectories of system (3.1), i.e.

$$\frac{\partial p_i}{\partial p_i} + \frac{\partial q^i}{\partial q^i} = \frac{\partial}{\partial p_i} \left( -\frac{\partial H}{\partial q^i} - \lambda^\alpha \frac{\partial \Phi_\alpha}{\partial q^i} \right) + \frac{\partial}{\partial q^i} \left( \frac{\partial H}{\partial p_i} + \lambda^\alpha \frac{\partial \Phi_\alpha}{\partial p_i} \right) = 0$$

This relation can be rewritten in the form

$$[\lambda^\alpha, \Phi_\alpha] = 0 \quad (3.5)$$

Here  $\lambda^\alpha$  are functions of the coordinates and momenta determined from the system of linear Eqs.(3.2). Eq.(3.5) by convention is identically satisfied and, consequently, imposes additional limitations on the possible choice of the functions  $\Phi_\alpha$ .

We will obtain an invariant measure on the layers  $H = \text{const}$ ,  $\Phi_\alpha = \text{const}$ . We will introduce the functions  $\Psi_\mu(x)$  ( $\mu = 1, \dots, m$ ,  $m = 2n - (k + 1)$ ) so that the quantities  $E = H(x, y)$ ,  $z_\alpha = \Phi_\alpha(x)$ ,  $\zeta_\mu = \Psi_\mu(x)$  can be regarded as curvilinear coordinates in phase space. The transformation of the coordinates  $x \rightarrow (\zeta, E, z)$  can be reversed and written in the form  $x^i = x^i(\zeta, E, z, y)$ . We will denote by  $\Delta$  the Jacobian of this transformation

$$\Delta = e_{i_1 \dots i_m j_1 \dots j_k} \frac{\partial x^{i_1}}{\partial \zeta_1} \dots \frac{\partial x^{i_m}}{\partial \zeta_m} \frac{\partial x^j}{\partial E} \frac{\partial x^{j_1}}{\partial z_1} \dots \frac{\partial x^{j_k}}{\partial z_k} \quad (3.6)$$

Here  $e_{i_1 \dots i_m j_1 \dots j_k}$  are the Levi-Civita symbols. Since the phase volume  $d^{2n}x$  is invariant under a shift along the trajectories, and  $dE, dz_1, \dots, dz_k$  are also invariable, we see from the equation  $d^{2n}x = \Delta d^m \zeta dE dz^k$  that  $\Delta d^m \zeta$  will be an invariant measure. It obviously does not change for any one-to-one change in the coordinates  $\zeta \leftrightarrow \zeta'$ . The time-averages for each function  $\varphi(x)$ , in view of the ergodicity, are identical with the average over the invariant measure

$$\langle \varphi(x) \rangle = \int \varphi \Delta d^m \zeta / \int \Delta d^m \zeta \quad (3.7)$$

Suppose the parameters  $y^a$  ( $a = 1, \dots, s$ ) vary slowly. We will obtain the rate of change of the energy of the system. We had from (3.1)

$$\frac{dH}{dt} = \frac{\partial H}{\partial y^a} \frac{dy^a}{dt} \quad (3.8)$$

Averaging Eq.(3.8) over time, we obtain, in view of the ergodicity of the system,

$$\frac{dE}{dt} = \left\langle \frac{\partial H}{\partial y^a} \right\rangle \frac{dy^a}{dt} \quad (3.9)$$

Eq.(3.9) can be proved rigorously using Anosov's averaging theorem [13].

We will show that Eq.(3.9) denotes the time-invariance of the quantity

$$\frac{\partial^k \Gamma(E, z, y)}{\partial z_1 \dots \partial z_k} = \int_0^E d^m \zeta \int dE \Delta \quad (3.10)$$

which has the meaning of the volume of the region situated on a  $(2n - k)$ -dimensional surfaces  $\Phi_\alpha(x) = z_\alpha$  and bounded by the surface  $H(x, y) \leq E$  (for simplicity we have assumed that the volume of the region  $H = 0$  is zero).

We will denote by  $\Delta_a$  the right-hand side of (3.6) in which the quantity  $\partial x^i / \partial E$  is

replaced by  $\partial x^i/\partial y^a$ . Since  $\partial x^i/\partial y^a + \partial x^i/\partial E \cdot \partial H/\partial y^a = 0$ , the equation  $\Delta_a = -\Delta \partial H/\partial y^a$  holds.

The following identity can be verified by direct substitution:

$$\partial \Delta/\partial y^a = \partial \Delta_a/\partial E \quad (3.11)$$

We will differentiate (3.10) with respect to  $y^a$ . Using (3.11) we have

$$\begin{aligned} \frac{\partial^{k+1}\Gamma(E, z, y)}{\partial z_1 \dots \partial z_k \partial y^a} &= \int d^{m_\zeta} \int_0^E dE \frac{\partial \Delta}{\partial y^a} = \int d^{m_\zeta} \int_0^E dE \frac{\partial \Delta_a}{\partial E} = \\ &= \int \Delta_a d^{m_\zeta} = - \int \Delta \frac{\partial H}{\partial y^a} d^{m_\zeta} \end{aligned} \quad (3.12)$$

Moreover, as follows from (3.10),

$$\frac{\partial^{k+1}\Gamma(E, z, y)}{\partial z_1 \dots \partial z_k \partial E} = \int \Delta d^{m_\zeta} \quad (3.13)$$

We can find the average  $\langle \partial H/\partial y^a \rangle$  using (3.7), (3.12) and (3.13)

$$\left\langle \frac{\partial H}{\partial y^a} \right\rangle = - \frac{\partial^{k+1}\Gamma(E, z, y)}{\partial z_1 \dots \partial z_k \partial y^a} / \frac{\partial^{k+1}\Gamma(E, z, y)}{\partial z_1 \dots \partial z_k \partial E} \quad (3.14)$$

The assertion follows from (3.9) and (3.14).

By defining the entropy of a system with constraints  $S(E, z, y)$  as  $\ln \partial^k \Gamma(E, z, y)/\partial z_1 \dots \partial z_k$ , i.e., the logarithm of the volume of the region on the surface  $\Phi_\alpha = z_\alpha$  bounded by the surface  $H(x, y) = E$ , we obtain Eq. (2.5).

*Note.* We can introduce the so-called conventional entropy for which Einstein's formula (1.2) holds (see /18, 19/). The definition of the conventional entropy is essentially equivalent to the postulation of Einstein's formula and the connection between the conventional entropy and the dynamics of the system is not completely clear.

We will now discuss how important are the assumptions made in deriving (2.5). If we dispense with the condition of the invariance of the phase volume (3.5), then in the case of the general position the quantity (3.10) would not be an adiabatic invariant; an adiabatic invariant can be constructed but the phase density  $\rho$  - the solution of the equation  $\partial(\rho p_i)/\partial p_i + \partial(\rho q^i)/\partial q^i = 0$ , would not occur in it, and relation (2.5) would look more complicated. Condition (3.3) is more important. Consider the simplest system for which this condition is not satisfied, namely, a system where the single constraint  $\Phi(x) = z$ . Note that the quantity  $[\Phi, H] \neq 0$ , unlike in the initial system, would be the additional integral  $\Phi = \text{const}$  and it would be ergodic on the surfaces  $H = \text{const}$ . We start the trajectory from a point on the surface  $H = E$ ,  $\Phi = z$ . In the case of a common position  $[\Phi, H] \neq 0$  at this point and since  $d\Phi/dt = [\Phi, H]$ , the trajectory descends from the surface  $\Phi = z$ . The trajectory remains on the surface only if the initial point lies on the submanifold  $[\Phi, H] = 0$ . Hence, we will return to the case with an even number of constraints  $\Phi_1 = \Phi = z$ ,  $\Phi_2 = [\Phi, H] = 0$ .

The problem arises as to how to connect the distribution function of one parameter with the entropy. This is obviously impossible to do using a relation of the type (2.5). One cannot see in all cases how to construct the corresponding auxiliary Hamiltonian of the system. However, one can always proceed as follows: in addition to the parameter  $\Phi_1$  being investigated, one introduces one more  $\Phi_2$  so that  $[\Phi_1, \Phi_2] \neq 0$  and Eq. (3.5) is satisfied (this can be done, for example, by determining  $\Phi_2$  from the equation  $[\Phi_1, \Phi_2] = 1$ ), and then obtaining the entropy  $S(E, z_1, z_2, y)$ , and from it, using Eq. (2.5), constructing the distribution function  $f(z_1, z_2)$ . By integrating the latter with respect to  $z_2$  we obtain the connection between the distribution function of the parameter  $z_1$  and the entropy.

**4. Example: a gas under a piston.** Consider an adiabatically insulated vessel with a gas, closed with a piston. A given force  $P$  acts on the piston. We will fix the coordinate  $a$  of the piston; it is required to obtain its distribution function. Using the procedure described above we will construct the distribution function of two quantities, one of which is the piston coordinate  $a$  and the other of which is the momentum of the piston  $A$ . The Hamilton function of the "gas + piston" system is  $G = H(p, q, a) + Pa + A^2/(2m)$ , where  $H(p, q, a)$  is the Hamilton function of the particles of the gas,  $m$  is the mass of the piston,  $H \geq 0$ ,  $P \geq 0$ ,  $a \geq 0$ . The motion of the system takes places on the surface  $G \equiv E$  in the phase space of the variables  $\{p, q, A, a\}$ . We will put  $\Phi_1 = a$ ,  $\Phi_2 = A$ , in which case  $[\Phi_1, \Phi_2] = 1$  and the system of Eqs. (3.2) takes the form  $\lambda^2 = -A/m$ ,  $\lambda^1 = -P - \partial H/\partial a$ ; conditions (3.5) are satisfied identically.

We will obtain the entropy of the system with specified values of  $\Phi_1$  and  $\Phi_2$ . To do this we must take a region  $G \leq E$  in a plane in the phase space  $\{p, q, A, a\}$ , defined by the equations  $a = a_0$ ,  $A = A_0$ , and calculate the logarithm of its volume  $\Gamma$ . The volume  $\Gamma$  is obviously equal to the volume of the region in the space of the variables  $\{p, q\}$  bounded by the surface

$H(p, q, a_0) = E - Pa_0 - A_0^2/(2m)$ . Hence, the entropy of the system with constraints can be expressed in terms of the entropy of the gas in the vessel  $S_g(E, a)$  using the formula  $S(E, a, A) = S_g(E - Pa - A^2/(2m), a)$ . From Eq. (2.5) we have

$$f(a, A) = \text{const} \frac{\partial}{\partial E} \exp S_g(E - Pa - A^2/(2m), a) \quad (4.1)$$

The distribution function of the coordinates of the piston can be found by integrating (4.1)

$$f(a) = \text{const} \int_0^{\sqrt{2m(E-Pa)}} \frac{\partial}{\partial E} \exp S_g(E - Pa - A^2/(2m), a) dA \quad (4.2)$$

Both formulas (4.1) and (4.2) hold for a large number of gas particles under the piston (classical gas dynamics), and also for a small number of particles. In the first case, we can obtain a Gaussian distribution from (4.2), in the second case it does not occur, and the fluctuations in the position of the piston will not be small, while the average value is not the same as the most probable value.

5. Variational principles for the distribution function. Consider a stationary point of the functional (the parameter  $y$  in the entropy is omitted)

$$I(E(z)) = \int \exp S(E(z), z) d^k z$$

on the set of functions  $E(z)$  and  $f(z)$ , which satisfy the conditions

$$\int E(z) f(z) d^k z = E, \quad \int f(z) d^k z = 1, \quad f(z) \geq 0 \quad (5.1)$$

The function  $f(z)$  corresponding to the stationary points of the functional  $I$  satisfies Eq. (2.5), as can easily be verified.

We will give the corresponding duality formulation. We will denote by  $R(\lambda, z)$  the Young-Fenchel function  $\exp S(E, z)$  of the energy  $E$

$$R(\lambda, z) = \sup_E (\lambda E - \exp S(E, z))$$

At the stationary point of the functional

$$\int R(\eta f(z), z) d^k z - E\eta$$

with respect to all numbers  $\eta$  and functions  $f(z)$  which satisfy the second constraint (5.1), Eq. (2.5) is satisfied.

The assertions formulated for systems in a thermostat reduce in the limit as  $n \rightarrow \infty$  to the principle of maximum uncertainty, well-known in statistical mechanics.

6. The principle of maximum entropy for Hamiltonian systems. In connection with the above the following question arises: can we state an analogue of Gibbs' principle (the principle of maximum entropy) for ergodic Hamiltonian systems for any choice of the parameters  $\Phi_\alpha$  and for finite  $n$ ? Below we give a positive answer to this question (in fact we discuss the stationarity of the entropy), but, in the corresponding variational principle, another entropy occurs - not the entropy of a system for fixed values of the parameters which occurs in Eq. (2.5), but the entropy of the system for fixed mean values of the parameters. For the latter, relation (2.5) does not occur.

We will impose the following constraint on the system with Hamiltonian function  $H(x, y)$ :

$$\frac{1}{\theta} \int_0^\theta \Phi_\alpha(x_t) dt = \bar{x}_\alpha \quad (6.1)$$

The equations describing this system have the form (3.1), where  $\lambda^\alpha$  are numbers found from conditions (6.1). When  $\theta$  changes, system (3.1) preserves its form, but the values of the numbers  $\lambda^\alpha$  change. If we allow  $\theta$  to tend to infinity, the left-hand side of (6.1) reduces to the mean value of the functions  $\Phi_\alpha$  along the trajectory  $\langle \Phi_\alpha \rangle$ , while the Lagrange multipliers  $\lambda^\alpha$  will be given by the equations

$$\langle \Phi_\alpha \rangle = \bar{x}_\alpha \quad (6.2)$$

We will assume that the hypersurfaces  $G \equiv H(x, y) + \lambda^\alpha (\Phi_\alpha(x) - \bar{x}_\alpha) = E$  are compact and bound a finite volume  $\Gamma(E, \lambda, \bar{x})$  (for simplicity the dependence of  $\Gamma(E, \lambda, \bar{x})$  on  $y$  is not indicated in the notation, since it is not important in what follows). This assumption specifies a certain region of permissible values of the constants  $\lambda^\alpha, \bar{x}_\alpha$ . We will denote by  $D$  the region of those values of  $\lambda^\alpha, \bar{x}_\alpha$  in which we also have  $\partial \Gamma / \partial E \neq 0$ .

Suppose the motion on the hypersurfaces  $G = \text{const}$  is ergodic. In the same way as for (3.12) we can prove the equations

$$\frac{\partial \Gamma(E, \lambda, \bar{z})}{\partial \lambda^\alpha} = - \int_{G=E} \frac{\Phi_\alpha(x) - \bar{z}_\alpha}{|\nabla_x G|} d\sigma, \quad \frac{\partial \Gamma(E, \lambda, \bar{z})}{\partial E} = \int_{G=E} \frac{d\sigma}{|\nabla_x G|} \quad (6.3)$$

In addition, according to the Birkhoff-Khinchin theorem

$$\langle \Phi_\alpha \rangle = \int_{G=E} \Phi_\alpha |\nabla_x G|^{-1} d\sigma / \int_{G=E} |\nabla_x G|^{-1} d\sigma \quad (6.4)$$

It can be seen from (6.3) and (6.4) that the relations for determining  $\lambda^\alpha$  (6.2) can be rewritten in the form  $\partial \Gamma(E, \lambda, \bar{z}) / \partial \lambda^\alpha = 0$ . Hence, the required values of  $\lambda^\alpha$  are stationary points of the function  $\Gamma(E, \lambda, \bar{z})$  with respect to  $\lambda^\alpha$ . We will assume that there is one stationary point  $\lambda_0(E, \bar{z})$ , in  $D$ , and we will determine the entropy of the system for fixed mean values of the parameters from the equation  $S(E, \bar{z}) = \ln \Gamma(E, \lambda_0(E, \bar{z}), \bar{z})$ . This quantity is obviously an adiabatic invariant.

The following variational principle holds: a stationary point of the entropy  $S(E, \bar{z})$  with respect to  $\bar{z}$  corresponds to the true mean values of the parameters  $\Phi_\alpha$ .

To prove this we note that the function  $\Gamma(E, \lambda, \bar{z})$  can be represented in the form  $\Gamma(E, \lambda, \bar{z}) = \Gamma_0(E + \lambda^\alpha \bar{z}_\alpha, \lambda)$ , where  $\Gamma_0(E, \lambda)$  is the volume of the region of phase space bounded by the surface  $H(x, y) + \lambda^\alpha \Phi_\alpha(x) = E$ . Hence, the equations for  $\lambda_0$  have the form

$$\left. \frac{\partial \Gamma_0}{\partial E} \bar{z}_\alpha + \frac{\partial \Gamma_0}{\partial \lambda^\alpha} \right|_{E + \lambda_0^\alpha \bar{z}_\alpha, \lambda_0} = 0 \quad (6.5)$$

We will write the condition for  $S(E, \bar{z})$  to be stationary with respect to  $\bar{z}$  as

$$\frac{1}{\Gamma} \left[ \frac{\partial \Gamma_0}{\partial E} \lambda_0^\alpha + \left( \frac{\partial \Gamma_0}{\partial E} \bar{z}_\beta + \frac{\partial \Gamma_0}{\partial \lambda^\beta} \right) \frac{\partial \lambda_0^\beta}{\partial \bar{z}_\alpha} \right] = 0 \quad (6.6)$$

It follows from (6.5) and (6.6) that at the stationary point with respect to  $\bar{z}$   $\lambda_0^\alpha = 0$ , hence  $G = H$ , and according to (6.4),  $\langle \Phi_\alpha \rangle$  is identical with the true mean values of  $\Phi_\alpha$  (i.e. along the trajectory of the initial system).

Bear in mind that the entropy for fixed mean values of the parameters, unlike the entropy for fixed values of the parameters, has meaning for any number of parameters (not necessarily even), in which case constraints of the type (3.5) are also unimportant.

#### REFERENCES

1. EINSTEIN A., Theory of opalescence in uniform liquids and liquid mixtures in the region of the critical state, collected Scientific Papers, 3, Nauka, Moscow, 1966.
2. GIBBS J., Thermodynamics. Statistical Mechanics, Nauka, Moscow, /Russian translation/, 1982.
3. HERTZ P., Uber die mechanischen Grundlagen der Thermodynamik, Ann. d. Phys. Vierte Folge, Bd.33, H.2, N.12; B.33, H.3, 13, 1910.
4. LANDAU L.D. and LIFSHITS E.M., Theoretical Physics, 5, Statistical Physics, Nauka, Moscow, 1964.
5. SINAI YA.G. and SHIL'NIKOV L.P. (Eds.), Strange Attractors, Mir, Moscow, 1981.
6. LIKHTENBERG A. and LIBERMAN M., Regular and Stochastic Dynamics, Mir, Moscow, 1984.
7. SINAI YA.G. (Ed.), Results of Science and Technology. Series on Modern Problems in Mathematics, 2, Dynamic Systems, VINITI, Moscow, 1985.
8. ZASLAVSKII G.M., Stochasticity of Dynamic Systems, Nauka, Moscow, 1984.
9. NEIMARK YU.I. and LANDA P.S., Stochastic and Chaotic Vibrations, Nauka, Moscow, 1987.
10. ULENBECK J. and FORD J., Lectures on Statistical Mechanics, Mir, Moscow, /Russian translation/, 1965.
11. WEBER R.H. and GANS R., Repertorium der Physik (bearbeitet von R.H. Weber und P. Hertz). B.1, 2. Leipzig, Teubner, 613, 1916.
12. LEVI-CIVITA T., Drei Vorlesungen uber adiabatischen Invarianten, Abb. Math. Sem. Univ. Hamburg, B.6, 1928.
13. ANOSOV D.V., Averaging in systems of ordinary differential equations with rapidly vibrating solutions, Izv. Akad. Nauk SSSR, Ser. Mat. 24, 5, 1960.
14. KASUGE T., On the adiabatic theorem for the Hamiltonian systems of differential equations in the classical mechanics, I, II, III, Proc. Japan. Acad. 37, 7, 1961.
15. TERLETSKII YA.P., Statistical Physics, Vyssh. Shkola, Moscow, 1966.
16. KUBO R., Statistical Mechanics, Mir, Moscow, 1967.



17. ARNOL'D V.I., KOZLOV V.V. and NEISHTADT A.I., Mathematical aspects of classical and celestial mechanics, Results of Science and Technology, Series on Modern Problems in Mathematics. Dynamic Systems. VINITI, Moscow, 1985.
18. KLIMONTOVICH YU.L., Statistical Physics, Nauka, Moscow, 1982.
19. STRATONOVICH R.L., Non-linear Non-equilibrium Thermodynamics, Nauka, Moscow, 1985.

Translated by R.C.G.

*PMM U.S.S.R.*, Vol.52, No.6, pp. 746-753, 1988  
Printed in Great Britain

0021-8928/88 \$10.00+0.00  
© 1990 Pergamon Press plc

## THE ASYMPTOTIC FORM OF THE STATIONARY SEPARATED CIRCUMFLUENCE OF A BODY AT HIGH REYNOLDS NUMBERS\*

S.I. CHERNYSHENKO

An asymptotic theory of the stationary separated circumfluence of bodies at high Reynolds numbers,  $Re$ , is constructed. It is shown that the length and width of the separated zone (SZ) is proportional to  $Re$  and that the drag coefficient is proportional to  $Re^{-1}$ . A cyclic boundary layer is located around the separated zone with a constant vorticity. In the scale of the body, the flow tends towards a Kirchhoff flow with a velocity on a free line of flow of the order of  $Re^{-1/2}$ , which satisfies the Brillouin-Villat condition.

A review of the attempts which have been made to describe the two-dimensional separated circumfluence of a body at high Reynolds numbers is given in /1, 2/. Certain features of the asymptotic structure of the solution based on qualitative arguments were pointed out in /3, 4/. The corresponding shape of the separated zone was calculated in /5/. However, no complete theory was constructed in these papers. The appearance of the numerical calculations in /6, 7/ stimulated further investigations and a model with a non-zero jump in the Bernoulli constant on the boundary of the separated zone was proposed in /8/. A number of hypotheses concerning the limiting structure of the flow were put forward in /9/.

In the solution obtained below the flow in the scale of the body is described as in /1, 2/ but the velocity is of the order of  $Re^{-1/4}$ . The flow characteristics in this zone are correspondingly renormalized. The flow in the scale of the separated zone corresponds to the assumptions made in /3, 4/. Unlike in /1-4/, the flow in the scale of the body is not directly combined with the flow in the scale of the separated zone. There are several embedded zones and the possibility of uniting these ensures the selfconsistency of the expansion. Moreover, the cyclic boundary layer on the boundary of the separated zone plays an important role.

1. Let us transform to dimensionless variables by employing the characteristic size of the body and the velocity at infinity as the scales. As  $Re \rightarrow \infty$ , let the length and width of the separated zone tend to infinity while remaining of the same order. Then, in the limit, the flow in the scale of the separated zone will be a vortex potential flow /10/. According to the Prandtl-Batchelor theorem, the vorticity is constant in the detached domains (Fig.1).

\**Prikl.Matem.Mekhan.*, 52,6,958-966,1988