symmetrical heating of cylindrical bodies," Izv. Vyssh. Uchebn. Zaved., Chern. Met., No. 6, 131-136 (1970).
4. V. G. Lisienko, V. V. Volkov, and B. I. Kitaev, "Numerical calculation of generalized angular coefficients in a system with complex geometry in the presence of absorbing media," Izv. Vyssh. Uchebn. Zaved., Chern. Met., No. 2, 151-155 (1974).
5. A. V. Bushinskii, "Determination of optical geometric coefficients of thermal radiation by the Monte Carlo method," Inzh.-Fiz. Zh., 30, No. 1, 160-166 (1976).
6. N. S. Bakhvalov, Numerical Methods [in Russian], Nauka, Moscow (1972).
7. R. Siegel and J. R. Howell, Thermal Radiation Heat Transfer, McGraw–Hill (1972).
8. I. R. Mikk, "Application of generalized angular coefficients in calculation of radiant heat exchange," Teplofiz. Vys. Temp., 1, No. 1, 128-135 (1963).

MODELING OF IRREVERSIBLE PROCESSES BY ANALOGY METHODS OF STATISTICAL MECHANICS

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Analogies to statistical mechanics of a Gibbs ensemble are constructed on the basis of the reflection method for dissipative macroscopic processes.

The formalism of classical and irreversible thermodynamics can be used successfully to construct mathematical models of a broad class of different processes, particularly control processes [1]. This is primarily due to the existence of a profound analogy between the equations of a whole range of dynamic systems and thermodynamics. The analogy between nonequilibrium thermodynamics and analytical mechanics was analyzed in detail in [2, 3], where it was shown that thermodynamic relations can be represented in the form of Lagrange or Hamilton equations. The basis for this formalism is an artificial method of introducing the so-called "mirror reflected system" with negative dissipation and decreasing entropy [4].

The Lagrangian of the total system, including the original and reflected parts, can be represented in the form

$$\mathcal{L} = \tilde{K}(\dot{x}_i^*,\ \dot{x}_i) - \frac{1}{2}R(\dot{x}_i^*,\ \dot{x}_i) + \frac{1}{2}R^*(\dot{x}_i^*,\ \dot{x}_i) - \tilde{V}(x_i^*,\ x_i). \tag{1}$$

Here the functions $\tilde{K}$, $\tilde{V}$, R, R* are constructed on the basis of specific expressions for the kinetic and potential energies and the dissipation function.

By means of [1] one can introduce the generalized momenta

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = \frac{\partial \tilde{K}}{\partial \dot{x}_i} - \frac{1}{2}\frac{\partial R}{\partial \dot{x}_i};\ p_i^* = \frac{\partial \mathcal{L}}{\partial \dot{x}_i^*} = \frac{\partial \tilde{K}}{\partial \dot{x}_i^*} + \frac{1}{2}\frac{\partial R^*}{\partial \dot{x}_i^*} \tag{2}$$

and the Hamiltonian

$$\mathcal{H} = p_i\dot{x}_i + p_i^*\dot{x}_i^* - \mathcal{L}. \tag{3}$$

Here and below doubly repeated subscripts imply summation. For an appropriate choice of the functions R and R*, $\mathcal{H}$ is an integral of motion.

For a system of material points, moving in a medium with a linear resistance law, the functions (1)-(3) are [4]

$$\mathcal{L} = a_{ik}\dot{x}_i^* x_k - \frac{1}{2}r_{ik}\dot{x}_i^* x_k + \frac{1}{2}r_{ik}\dot{x}_i x_k^* - b_{ik}x_i^* x_k, \tag{4}$$

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$$\mathcal{H} = a_{ik}\dot{x}_i^*\dot{x}_k + b_{ik}x_i x_k = a_{ik}^{-1}\left(p_i + \frac{1}{2}r_{im}x_m^*\right)\left(p_k^* - \frac{1}{2}r_{km}x_m\right) - b_{ik}x_i^* x_k, \tag{5}$$

$$p_i = a_{ik}\dot{x}_k^* - \frac{1}{2}r_{ik}x_k^*, \quad p_i^* = a_{ik}\dot{x}_k + \frac{1}{2}r_{ik}x_k.$$

The matrix elements a_{ik}, b_{ik}, r_{ik} are the coefficients of the **quadratic forms of the** kinetic $K = \frac{1}{2}a_{ik}\dot{x}_i\dot{x}_k$ and potential $V = \frac{1}{2}b_{ik}x_i x_k$ energies, and the dissipative function $D = \frac{1}{2}r_{ik}\dot{x}_i\dot{x}_k$.

The same formalism can be used in nonequilibrium thermodynamics [2]. For a thermodynamic system whose state is described by the set of parameters $\{x_i\}$, in the case of purely dissipative processes ($\tilde{K} = 0$) the functions (1)-(3) are

$$\mathcal{L} = \frac{1}{2}L_{ik}^{-1}(\dot{x}_i^* x_k - x_i^*\dot{x}_k) - g_{ik}x_i^* x_k, \tag{6}$$

$$\mathcal{H} = \frac{1}{2}g_{ik}x_i^* x_k + 2g_{ik}L_{kl}L_{im}p_l^* p_m, \tag{7}$$

$$p_l^* = \frac{1}{2}L_{lk}^{-1}x_k, \quad p_m = -\frac{1}{2}L_{mk}^{-1}x_k^*, \tag{8}$$

where g_{ik} are the matrix elements of the coefficients of the **quadratic form, being** the series expansion of the entropy in deviations $\{x_i\}$ of the parameters from their **equilibrium values,** $g_{ik} = \partial^2 S/\partial x_i \partial x_k$.

Using the Hamiltonian $\mathcal{H}$ and (5), (7), one can write the **system of canonical** Hamiltonian equations

$$\dot{p}_i^* = -\frac{\partial\mathcal{H}}{\partial x_i^*}, \quad \dot{x}_i^* = \frac{\partial\mathcal{H}}{\partial p_i^*}, \quad \dot{p}_i = -\frac{\partial\mathcal{H}}{\partial x_i}, \quad \dot{x}_i = \frac{\partial\mathcal{H}}{\partial p_i}. \tag{9}$$

In the present work the Hamilton formalism considered **above is used to construct** the statistical mechanics of dissipative systems and corresponding analogies for **irreversible thermodynamic** processes.

Consider the statistical ensemble in the phase space of **generalized coordinates** and momenta x_i, x_i^*, p_i, p_i^* of the total system. Due to the existence of relation (9) **one can write the Gibbs**–Liouville equation for the distribution function $F(x_i, x_i^*, p_i, p_i^*)$ in the form [5]

$$i\frac{\partial F}{\partial t} = \hat{L}F, \tag{10}$$

where $i = (-1)^{1/2}$, and

$$\hat{L} = -i\left[\left(\frac{\partial\mathcal{H}}{\partial p_i}\frac{\partial}{\partial x_i} - \frac{\partial\mathcal{H}}{\partial x_i}\frac{\partial}{\partial p_i}\right) + \left(\frac{\partial\mathcal{H}}{\partial p_i^*}\frac{\partial}{\partial x_i^*} - \frac{\partial\mathcal{H}}{\partial x_i^*}\frac{\partial}{\partial p_i^*}\right)\right]. \tag{11}$$

The nonstationary solution of Eq. (10) can be represented **by an expansion** of F in a Fourier series of eigenfunctions of the Liouville operator $\hat{L}$ [5].

Standard calculations show that $dF/dt = 0$, i.e., F is an **integral of motion** along the phase trajectory. For stationary ensembles the Hamiltonian $\mathcal{H}$ (3), (7) is also **an integral of motion.** Therefore, according to the general ideas of statistical physics [6] the distribution **function can be presented** in the form

$$F = \exp(\alpha\mathcal{H} + c). \tag{12}$$

The constant c is found from the normalization condition, **and α is determined** by the specific physical content of the problem.

Thus, the function (12) is the analog of the Gibbs **canonical distribution, and** describes both the ensemble of mechanical particle systems in the presence of friction, **and the ensemble of** thermodynamic systems undergoing irreversible processes. Various mean-statistical **quantities can be calculated** on the basis of the distribution function (12) by the apparatus of statistical physics [5]. **Application of the** apparatus of statistical mechanics to ensembles of macroscopic thermodynamic systems **may seem artificial** at first glance. It can be quite useful, however, in the mathematical modeling of a **wide class of technological** processes, particularly those used for heterogeneous systems. Various local **fluctuations, related to the** inhomogeneity of hydrodynamic, temperature, and concentration fields, occur in these **systems. This is** precisely related to the necessity of applying statistical methods [7].

As an example of using the distribution function (12) **for a mechanical** dissipative system we consider the ensemble of local pulsating particle motions of a **suspended layer. In the** stationary regime the pseudofluidized dissipating power is compensated by the continuous energy supply from the mean flow to large-scale motions and further to small-scale fluctuations at which the dissipation process occurs.

According to the method discussed above we replace the carrying current of the associated system. Since the particle interaction with the flow occurs at the particle surface, we can put $x_i = x_i^*$ in Eqs. (1)-(5). In this case the system becomes self-oscillating or "quasiconservative". Its Hamiltonian in a Cartesian coordinate system equals, according to (1), (3), and (5)

$$\mathcal{H} = 2H = 2(K + V) = 2\left[\sum_i \frac{p_i p_i}{2m} + V(x_1 \ldots x_n)\right], \tag{13}$$

and the distribution function (12) is

$$F = \exp\left\{\frac{-H + \tilde{F}}{\theta}\right\}, \tag{14}$$

where $H = K + V$ means the total particle energy; $\tilde{F} = c\theta$, $\theta = -(2\alpha)^{-1}$, distribution parameters; and p_i, particle momentum.

Integrating (13) over the spatial coordinates x_i and over the velocities of all particles except one, we reach a Maxwell distribution in one-particle velocities

$$F(v_i) = \left(\frac{m}{2\pi\theta}\right)^{3/2} \exp\left[-\frac{mv^2}{2\theta}\right], \tag{15}$$

which was used in constructing an approximate statistical theory of a suspended layer [8].

The Gibbs–Liouville Eq. (10) can be simplified in the case of purely dissipative processes, for which relations (6)-(8) occur. Since in this case there is no analog to kinetic energy ($\tilde{K} = 0$, $K = 0$), the generalized momenta are linear combinations of the generalized coordinates (8), and they can be eliminated, transforming from the distribution function $F(x_i, x_i^*, p_i, p_i^*)$ to the distribution $f(x_i, x_i^*)$ in space coordinates. Formally this can be obtained by integrating (10) over momenta. Taking into account the obvious relation

$$f(x_i, x_i^*) = \int_{\Gamma_p} F(x_i, x_i^*, p_i, p_i^*)\, d\Gamma_p, \tag{16}$$

where $d\Gamma_p = dp_1 \ldots dp_n dp_1^*$, but the integration is performed over the whole variable range Γ_p, after standard transformations [9] (10) acquires the form

$$\frac{\partial f}{\partial t} + \dot{x}_i \frac{\partial f}{\partial x_i} + \dot{x}_i^* \frac{\partial f}{\partial x_i^*} = 0. \tag{17}$$

Phenomenological relations can be written down for the quantities $\dot{x}_i$, $\dot{x}_i^*$

$$\dot{x}_i = -L_{ik} X_k (x_1 \ldots x_n), \quad \dot{x}_i^* = L_{ik} X_k^* (x_1^* \ldots x_n^*), \tag{18}$$

where X_k, X_k^* play the role of thermodynamic forces. The function $f(x_i, x_i^*)$ retains the property of integral of motion. The solution of Eq. (17) can be represented in the form

$$f(x_i, x_i^*) = \sum_k c^k \exp \sum_i \left[-a_i^k x_i - a_i^{*k} x_i^* + \int_0^t (a_i^k \dot{x}_i + a_i^{*k} \dot{x}_i^*)\, dt\right]. \tag{19}$$

The constants c_i^k, a_i^k, a_i^{*k} are determined by the initial conditions and by the normalization. It is seen from the solution (19) that for the evolution time of the distribution function a distinctive regular regime is possible, for which only one term is important in the sum over k, starting at some moment of time. Besides, it is possible, in principle, to eliminate the parameter x_i^* of the reflected system. In analogy with (16), integrating over the region Γ_{x^*} of variation of x_i^*, we have

$$f(x_i) = \int_{\Gamma_{x^*}} f(x_i, x_i^*)\, d\Gamma_{x^*} = \sum_k A^k \exp \sum_i \left(-a_i^k x_i + \int_0^t a_i^k \dot{x}_i dt\right). \tag{20}$$

This function satisfies the equation

$$\frac{\partial f}{\partial t} + \dot{x}_i \frac{\partial f}{\partial x_i} = 0. \tag{21}$$

The latter relations were used to describe the evaporation process of a polydisperse system of drops [10].

Consider a stationary solution of Eq. (17), Following [6], we introduce the generating function of the total system

$$\varphi = \frac{1}{2} L_{ik}^{-1} (\dot{x}_i^* \dot{x}_k^* + \dot{x}_i \dot{x}_k). \tag{22}$$

Hence we find

$$\begin{gathered} \dot{x}_i = L_{ik} \frac{\partial \varphi}{\partial \dot{x}_k} = - L_{ik} X_k = - L_{ik} g_{kl} x_l, \\ \dot{x}_i^* = L_{ik} \frac{\partial \varphi}{\partial \dot{x}_k^*} = L_{ik} X_k^* = L_{ik} g_{kl} x_l^*. \end{gathered} \tag{23}$$

By means of (23) the stationary equation (17) is transformed to the form

$$x_i^* \frac{\partial f}{\partial x_i^*} - x_i \frac{\partial f}{\partial x_i} = 0. \tag{24}$$

We choose $f(x_i, x_i^*)$ in the form

$$f(x_i, x_i^*) = \exp \frac{\alpha}{2} (- L_{ik} g_{kl} x_l x_i + L_{ik} g_{kl} x_l^* x_i^*). \tag{25}$$

It satisfies Eq. (24) if $S = 2\varphi = 0$. The latter condition is satisfied, since entropy production in the basic system is compensated by its decrease in the reflected one. Integrating (25) over the coordinates of the reflected system, we obtain a distribution function for the original system

$$f_1(x)_i = A \exp \left(- \frac{1}{2} \alpha L_{ik} g_{ik} x_k x_i \right) = A \exp(- \alpha D(x_i)), \tag{26}$$

where $D(x_i)$ is the dissipative function.

The same result was obtained in [7] by the method of the Jaynes formalism [7]. We note that (17) is a special case of the continuity equation

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_i} (\dot{x}_i f) + \frac{\partial}{\partial x_i^*} (\dot{x}_i^* f) = 0. \tag{27}$$

For real systems ($x_i^* = 0$) it was used many times in the one-dimensional case to describe the evolution of the distribution of polydisperse systems over the radius in mass exchange processes [10, 12, 13]. Effective methods of solving Eq. (27) with nonlinearities due to the kinetic process were developed in [12]. These methods can also be used in solving the Gibbs–Liouville Eq. (10). The quantities $\dot{x}_i f$ and $\dot{x}_i^* f$, appearing under the divergence sign, can be considered as generalized flows, obeying the phenomenological laws [14]:

$$J_i = \dot{x}_i f = - L \frac{\partial \mu(f)}{\partial x_i}, \; J_i^* = \dot{x}_i^* f = L \frac{\partial \mu(f)}{\partial x_i^*}, \tag{28}$$

where $\mu(f)$ is the chemical potential for configuration f in phase space. Introducing the diffusion coefficient D_x:

$$\begin{gathered} J_i = - L \frac{\partial \mu}{\partial f} \frac{\partial f}{\partial x_i} = - D_x \frac{\partial f}{\partial x_i}, \\ J_i^* = L \frac{\partial \mu}{\partial f} \frac{\partial f}{\partial x_i^*} = D_x \frac{\partial f}{\partial x_i^*}, \end{gathered} \tag{29}$$

we transform (27) into a diffusion equation in phase space

$$\frac{\partial f}{\partial t} = D_x \left(\frac{\partial^2 f}{\partial x_i \partial x_i} - \frac{\partial^2 f}{\partial x_i^* \partial x_i^*} \right). \tag{30}$$

A similar equation for real systems is used in analyzing random walk and in the theory of Brownian motion [15].

If instead of D_x one uses the operator representation of the diffusion coefficient $\hat{D} = D_x (1 + \tau \, \partial/\partial t)^{-1}$ [16], making it possible to take into account the presence of some additional relaxation process in the system, instead of (30) we obtain a diffusion equation of more general form:

$$\frac{\partial f}{\partial t}+\tau\frac{\partial^2 f}{\partial t^2}=D_x\left(1+\tau\frac{\partial}{\partial t}\right)\left(\frac{\partial^2 f}{\partial x_i\partial x_i}-\frac{\partial^2 f}{\partial x_i^*\partial x_i^*}\right). \tag{31}$$

By the methods considered in [14] one can obtain analogies for the Fokker–Planck equations of rotational diffusion, and so on.

Thus, the formalism considered in this paper can be useful in modeling a wide class of different macroscopic processes.

NOTATION

x_i and x_i^*, generalized coordinates of the initial and reflected systems; $\tilde{K}$, $\tilde{V}$, R, R^*, functions appearing in the Langrangian $\mathcal{L}$ (1); p_i, p_i^*, generalized momenta; $\mathcal{H}$, generalized Hamiltonian; $\dot{x}_i$, $\dot{x}_i^*$, generalized velocities (flows); K, V, D, a_{ik}, b_{ik}, r_{ik}, kinetic and potential energies, the dissipative function and matrix elements of the corresponding quadratic forms; L_{ik}, matrix elements of the phenomenological cioefficients; S, system entropy; L, Liouville operator; $F(x_i, x_i^*, p_i, p_i^*)$, distribution functions in the phase space of the appropriate variables; H, Hamiltonian of the mechanical conservative system; m, particle mass; φ, generating function defined in (22); J_i, J_i^*, thermodynamic flows; D_x, diffusion coefficient for phase space, τ, relaxation time; *, conjugate system; and $\cdot$, time differentiation.

LITERATURE CITED

1. B. N. Petrov, G. M. Ulanov, I. I. Gol'denblat, and S. V. Ul'yanov, Theory of Models in Control Processes [in Russian], Nauka, Moscow (1978).
2. I. F. Bakhareva, "Mechanical analogies of nonequilibrium thermodynamics," Zh. Fiz. Khim., 41, No. 7, 1717-1722 (1967).
3. I. F. Bakhareva, "Variational principles of nonequilibrium thermodynamics," Inzh.-Fiz. Zh., 20, No. 6, 1105-1110 (1971).
4. P. M. Morse and H. Feshbach, Methods of Theoretical Physics, Part 1, McGraw–Hill, New York (1953).
5. I. Prigogine, Nonequilibrium Statistical Mechanics, Interscience, New York (1962).
6. L. D. Landau and E. M. Lifshitz, Statistical Physics, Part 1, Pergamon Press (1980).
7. I. N. Taganov, Modeling of Mass and Energy Transfer Processes [in Russian], Khimiya, Leningrad (1979).
8. Yu. A. Buevich, "Approximate statistical theory of a suspended layer," Zh. Prikl. Mekh. Teor. Fiz., No. 6, 35-47 (1966).
9. A. Likhtenberg, Particle Dynamics in Phase Space [in Russian], Atomizdat, Moscow (1972).
10. G. P. Yasnikov, "Kinetics of the self-similar evaporation regime of a polydisperse drop system," Inzh.-Fiz. Zh., 42, No. 2, 243-250 (1982).
11. M. Traibus, Thermostatics and Thermodynamics [in Russian], Énergiya, Moscow (1970).
12. Yu. A. Buevich, "Kinetics of mass transfer of a polydisperse particle system with the surrounding medium," Zh. Prikl. Mat. Tekh. Fiz., No. 1, 50-57 (1966).
13. O. M. Todes, Yu. Ya. Kaganovich, S. P. Nalimov, et al., Dehydration of Solutions in a Boiling Layer [in Russian], Metallurgiya, Moscow (1973).
14. S. R. de Groot and P. Mazur, Nonequilibrium Thermodynamics, North-Holland, Amsterdam (1962).
15. S. Chandrasekhar, Stochastic Problems in Physics and Astronomy [Russian translation], IL, Moscow (1947).
16. G. P. Yasnikov, L. G. Gal'perin, and Z. N. Kutyavin, "Hyperbolic diffusion equation in a dispersive and relaxing medium," Inzh.-Fiz. Zh., 39, No. 2, 334-338 (1980).