PHYSICO-CHEMICAL PRINCIPLES OF MATERIALS DEVELOPMENT

# Simulating the Heat Conduction and Diffusion Processes in Methods for Generating and Processing Materials with Using Intense Energy Sources

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**Abstact**—A semiphenomenological model of the transport processes under the action of power energy sources is proposed. To explain the observed deviations of the linear system response to an external perturbation in the transport processes induced by intense energy fluxes, it is proposed to take into account the effect of inertia of the medium. The semiphenomenological model of processes is reduced to a system with two basis states. The techniques of the theory of microscopic objects for the solution of the system are applied. It is shown that the inertia of the medium is due to the finite time of establishing the equilibrium between the basis states.

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## **INTRODUCTION**

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The development of the technologies for obtaining and generating new materials based on the use of intense energy fluxes [1-3] leads to the problem of taking the inertia of the medium into account in the transport processes, that is, of describing these processes beyond the hydrodynamic scale under failure of the local quasiequilibrium principle. Lately, the interest in this problem has been in using the radiation of lasers with picoseconds and femtosecond pulse duration to study the process of heat transport in films and thin-layer structures [4-6].

It is believed [4-10] that the semiphenomenological approach allows the problem to be solved by the introduction of the small time  $\tau$  into the expression for the flux, which characterizes the relaxation effect on the small time scale, and the further transition to the hyperbolic transport equation. Although such a way of considering the inertia of the medium has long been known, its application leads to the loss of the laws of conservation [11]. Consequently, the behavior of the resulting equations is unknown.

These difficulties are caused by the fact that both small and large time scales take part in describing the transport process in the hyperbolic transport equation, as opposed to the microscopic approach, wherein rapid temporal fluctuations on the hydrodynamic scale are averaged and excluded from consideration [12]. As the conservation law, the continuity equation applied to the transition between the relaxation expression for the flux [13] and the hyperbolic transport equation covers not any relationship between the flux and the time. These difficulties can be removed by the current method, which uses the difference between the solutions of the second-order equation and the associated first-order equation with the matrix coefficients such that each component of this solution satisfies the initial equation.

The purpose of the present paper is to simulate the influence of the inertia of the medium on the transport processes occurring under the action of intense energy fluxes.

### INDIVIDUAL TRANSPORT PROCESSES

We use the coordinate representation to construct a model. For simplicity, let us restrict ourselves to the process of heat (mass) transport in solids. We use the probabilistic interpretation of the solution to decrease the number of dimensional variables. Then, the semi- 2 phenomenological transport equation for the reduced description of these processes in the superposition state  $\langle \mathbf{n} | = n_1 \langle 1 | + n_2 \langle 2 |$  [14] has the following form:

$$\frac{\partial \mathbf{n}}{\partial t} = \mathbf{H}\mathbf{n}, \quad \mathbf{H} = \Gamma - \mathbf{V}\frac{\partial}{\partial x},$$
$$\mathbf{\Gamma} = \Gamma \begin{pmatrix} -1 & 1\\ 1 & -1 \end{pmatrix}, \quad \mathbf{V} = V_0 \begin{pmatrix} -1 & 0\\ 0 & 1 \end{pmatrix}, \quad (1)$$
$$\mathbf{n} = \begin{pmatrix} n_1(t, x)\\ n_2(t, x) \end{pmatrix}, \quad t \ge 0,$$

where  $n_{1,2}(t, x)$  is the probability density of finding the system in states  $\langle 1 |$  and  $\langle 2 |$ ;  $\Gamma$  is the frequency of system transition between the states;  $V_0 = (B/\tau)^{1/2}$  is the limiting velocity of the transition; and  $\tau = 1/2\Gamma$  and B = 3 (*a*, *D*) are the kinetic coefficients of thermal diffusivity and diffusion.

The presence of the off-diagonal matrix elements in this equation means the existence of system transitions between the different basis states. Note that the equality between the off-diagonal matrix elements in (1) and the equality (or complex conjugation) of the 4 off-diagonal Hamiltonian matrix elements have the same physical meaning: the probability of finding the system in even one basis state  $N_{1,2}(t)$  should be constant in time.

To go into the entropy representation, we extract the velocity and kinetic balance matrices V and  $\Gamma$  and write Eq. (1) in the form of the continuity equation

$$\mathbf{n}'_t + (\mathbf{V}\mathbf{n})'_x = \Gamma\mathbf{n}.$$
 (2)

After the substitution  $d\mathbf{s} = Gd\mathbf{n}$ , we reduce Eq. (2) to the continuity equation for the vector function  $\mathbf{s} = \mathbf{s}(t, x)$ :

$$\mathbf{s}'_t + (\mathbf{V}\mathbf{s})'_x = \sigma\mathbf{s}, \quad \sigma = \Gamma + X_i\mathbf{V},$$
 (3)

where  $G = (T^{-1}, -\mu/T)$  is the thermodynamic multi-5 plier eatablishing the relationship between the heat (diffusion) process and the entropy density,  $X_i = (\ln |G|)'_x$  is the thermodynamic force, *T* is the temperature, and  $\mu$  is the chemical potential of the diffusing component.

After performing the Fourier transform over the variable x in (3), we move to the equation for the function  $\hat{\mathbf{s}}(t, \varsigma)$ . Setting  $\varsigma = 0$  and denoting  $\mathbf{S}(t) = \hat{\mathbf{s}}(t, 0)$ , we obtain the equation describing the process (1) in the entropy representation for the integral change in the vector function  $\sigma(t, x)$ :

$$\dot{\mathbf{S}} = \sigma \mathbf{S},\tag{4}$$

where  $\sigma$  is the entropy source of the process in the superposition state  $\langle \mathbf{S} | = S_1 \langle 1 | + S_2 \langle 2 |, X = (\ln |G|)'_x$  is the thermodynamic force, and  $G = (T^{-1}, -\mu/T)$  is the thermodynamic multipliers of the thermal and difffusion processes.

We consider that Eq. (1) describes the transitions between states  $\langle 1 |$  and  $\langle 2 |$  and allows one to bring the processes occurring in the large and small time scales into correspondence. To describe these processes, we go to the stationary basis states, wherein the system transitions between the basis states are absent. In this case, the system in one stationary state can be observed in another one. After performing the canonical transformation  $\mathbf{H} = \mathbf{U}_n \mathbf{L} \mathbf{U}_n^{-1}$ ,  $\boldsymbol{\sigma} = \mathbf{U}_S \mathbf{L} \mathbf{U}_S^{-1}$  and denoting  $\mathbf{n}_{st} = \mathbf{U}_n^{-1} \mathbf{n}$  and  $\mathbf{S}_{st} = \mathbf{U}_n^{-1} \mathbf{S}$  for states  $\langle \mathbf{I} |$  and  $\langle \mathbf{II} |$ , we obtain

$$\frac{\partial \mathbf{n}_{st}}{\partial t} = \mathbf{L}\mathbf{n}_{st}, \qquad (5)$$
$$\mathbf{n}_{st} = \begin{pmatrix} n_{-}(t,x)\\ n_{+}(t,x) \end{pmatrix}; \quad \mathbf{L}_{i} = \begin{pmatrix} \hat{L}_{-} & 0\\ 0 & \hat{L}_{+} \end{pmatrix},$$
$$\hat{L}_{\mp} = -\Gamma(1 \mp \sqrt{1 + (h\partial/\partial x)^{2}}), \quad h = \frac{V_{0}}{\Gamma},$$
$$\hat{\mathbf{S}}_{st} = \Omega \mathbf{S}_{st}, \qquad (6)$$
$$\mathbf{S}_{st} = \begin{pmatrix} \mathbf{S}_{+}(t)\\ \mathbf{S}_{-}(t) \end{pmatrix}, \quad \Omega_{i} = \begin{pmatrix} \Omega_{+} & 0\\ 0 & \Omega_{-} \end{pmatrix},$$

$$\Omega_{\pm} = \Gamma(-1 \pm \sqrt{1 + (hX)^2}).$$

Equations (5) and (6) describe the irreversible process in the stationary state  $\langle \mathbf{n}_{st} | = n_{-} \langle \mathbf{I} | + n_{+} \langle \mathbf{II} |$  and  $\langle \mathbf{S}_{st} | = S_{+} \langle \mathbf{I} | + S_{-} \langle \mathbf{II} |$  for the coordinate and entropy representations, respectively. They make it possible to consider the macroscopic and microscopic processes as a unified fluctuation process, where the fluctuation and dissipative properties appear according to the selected time scale. In them, the kinetic balance matrix  $\Gamma$  provides the performance of the heat (mass) and entropy conservation laws for the system in the thermodynamic equilibrium state (X = 0):

$$\int_{-\infty}^{\infty} (n_1(t,x) + n_2(t,x)) dx = \int_{-\infty}^{\infty} n_-(t,x) dx = 1,$$

$$(S_+(t) + S_-(t)) = S_+, \quad \dot{S}_+ = 0,$$
(7)

After denoting the Fourier transform of the vector function  $\hat{\mathbf{n}}(t, \varsigma)$  at  $\zeta = 0$  and  $\mathbf{S}(t, X)$  at X = 0 as  $\psi$ , we obtain  $d\psi/dt = \Gamma\psi$ . Hence, we find the equality from which the conservation laws (7) follow:

$$\psi(t) = \exp(\Gamma t)\psi_0 = (\operatorname{Pexp}(\mathbf{R}t))\psi_0^{\mathrm{st}},$$
$$\psi_0^{\mathrm{st}} = \mathbf{P}^{-1}\psi_0,$$

where  $\psi_0$  and  $\psi_0^{st}$  are the initial conditions for the vector functions  $\psi(t)$  and  $\psi_{st}$  in the superposition and stationary states respectively; **R** is the diagonal form of the  $\Gamma$  matrix; and **P** and **P**<sup>-1</sup> are the matrix of eigenvectors and its inverse.

The  $n_+(t, x)$  and  $S_-(t)$  solutions for stationary state  $\langle II|$  on the small time scale do not take part in the conservation laws (7) and are not observable in the experiment.

In order to establish the role of the metric, we consider the processes on the large time scale in stationary state  $\langle I |$ . Using the relation  $V = d\Omega_+/dX$  for the transport velocity, we obtain

$$V = V_0 \left(\frac{hX}{\sqrt{1 + (hX)^2}}\right).$$

that is, the transport process in state  $\langle I |$  takes place on the linear paths x = Vt, and it has the limiting value  $V_0$  $(X \longrightarrow \infty)$  only on them. In the experiment, the paths in the form of  $x = o(\sqrt{t})$  and the ones close to them are more characteristic. Since the first terms of the expansion of the  $\hat{L}_{-} \approx B\partial_x^2 - \tau (B\partial_x^2)^2$  operator in a series make the main contribution to the solution of (5), the results of studying the deviations from the hydrodynamic description of the transport processes under the action of intense energy fluxes allow one to prove the influence of the small-scale processes experimentally and to determine the frequency  $\Gamma = 1/2\tau$  of the system transition between basis states  $\langle 1 |$  and  $\langle 2 |$ .

The other case arises for the small-scale process occurring in stationary state (II). It restricts the application of the laws of conservation and the second law of thermodynamics. The irreversible process in state  $\langle II|$  follows the process in state  $\langle I|$  specularly. Although this process is not observed, we cannot eliminate it according to the physical sense; i.e., the solutions for both states are equivalent at  $t \rightarrow \infty$ . However, the process in state  $\langle II |$  occurs with an entropy decrease, being opposite to the dissipation process. The values  $\Omega_{-}$  $-2\Gamma$  define the size of the "gap" between the states with the positive and negative values of  $\Omega$ . In stationary state  $\langle II |$ , the system is open and is in contact with a thermostat, which induces the fluctuations in the system. Here, a feature of the approach comes into view [14]. According to this approach, the small-scale process similar to the microobject cannot be considered separately, excluding its interaction with the environment.

Note that the solutions  $n_{1,2}(t, x)$  and  $n_{\pm}(t, x)$  (any component of the vector functions *n* is generally rotation-independent) satisfy the hyperbolic equation

$$\hat{L}n_{1,2} = 0, \quad \hat{L} = \tau \partial^2 / \partial t^2 + \partial / \partial t - B \partial^2 / \partial x^2$$

Thus, even though the fact that the conservation law is absent in this equation is neglected, the number of possible solutions is too large to describe the relationship observed in the experiment. These solutions describe no oscillating processes in the local-nonequilibrium systems.

#### **RELATED TRANSPORT PROCESSES**

Up to now, the inertia of the medium was taken into account for the individual transport processes. The first and, probably, unique paper [15] considering the transport processes with the cross effects taken into account is based on the entropy representation of these processes using the relaxation expression for the flux [13] and on the formalism of the theory of irreversible processes, which is developed for the hydrodynamic scale. Therefore, the loss of the conservation laws occurs upon the transition from the entropy representation to the coordinate one. To provide the fulfillment of the conservation laws, we use the coordinate representation, which should lead to the representation of the entropy source in a quadratic form of the thermodynamic forces (fluxes) on the hydrodynamic scale under the right choice of the elements of the matrix coefficients [16]. For simplicity, we restrict ourselves to the case of the related heat and mass transport processes 1 and 2 in solids. Then, the semiphenomenological transport equation 2 giving the reduced description of these processes in the superposition state takes the form

$$\frac{\partial \mathbf{n}}{\partial t} = \mathbf{H}\mathbf{n}, \quad \mathbf{n} = \mathbf{n}(t, x), \quad t \ge 0,$$
 (8)

where  $\mathbf{H} = \begin{pmatrix} \mathbf{H}_{11} & \mathbf{H}_{12} \\ \mathbf{H}_{21} & \mathbf{H}_{22} \end{pmatrix}$  is the block-type differential

matrix operator;

$$\mathbf{H}_{ij}\left(\frac{\partial}{\partial x}\right) = \Gamma_{ij} - \mathbf{V}_{ij}\frac{\partial}{\partial x},$$
$$\mathbf{n} = \begin{pmatrix}\mathbf{n}_{1}\\\mathbf{n}_{2}\end{pmatrix}, \quad \mathbf{n}_{i} = \begin{pmatrix}n_{1}(t,x)\\n_{2}(t,x)\end{pmatrix},$$
$$\mathbf{V}_{ij} = V_{0}^{(ij)}\left(\begin{array}{c}-1 & 0\\0 & 1\end{array}\right),$$
$$\Gamma_{ij} = \Gamma_{ij}\left(\begin{array}{c}-1 & 1\\1 & -1\end{array}\right), \quad i \neq j,$$
$$\Gamma_{ij} = 0, \quad i \neq j, \quad (i,j) = 1, 2,$$

 $\mathbf{n}_i$  is the two-component vector function describing processes 1 and 2;  $\mathbf{H}_{ij}$  are the block elements of the **H** operator with the diagonal elements i = j describing the separate transport processes and the off-diagonal

elements describing the cross effects;  $V_0^{(ij)} = \left(\frac{B_{ij}}{\tau_{.}}\right)^{1/2}$  is

the limiting transport velocity, which is independent of the external perturbation;  $\tau_i = (2\Gamma_{ii})^{-1}$  is the small time characterizing the small scale; and  $B_{ij}$  are the kinetic coefficients measured in quasiequilibrium experimen-1 tal conditions for the diagonal (individual) (i = j) and off-diagonal (cross) ( $i \neq j$ ) processes.

The transition to the entropy representation is similar to the one described for the individual processes. Extracting the velocity and kinetic balance matrices V and  $\Gamma$ , we go to the continuity equation

$$\mathbf{n}_t' + (\mathbf{V}\mathbf{n})_x' = \Gamma \mathbf{n},\tag{9}$$

and, making the substitution  $d\mathbf{s} = \mathbf{G}d\mathbf{n}$ , we reduce Eq. (9) to the continuity equation for the vector function  $\mathbf{s} = \mathbf{s}(t, x)$ 

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$$\mathbf{s}'_t + (\overline{\mathbf{V}}\mathbf{s})'_x = \sigma \mathbf{s}, \quad \sigma = \Gamma + \mathbf{X}\overline{\mathbf{V}},$$
 (10)

where  $\mathbf{X} = \begin{pmatrix} \mathbf{X}_1 & 0 \\ 0 & \mathbf{X}_2 \end{pmatrix}$ , and  $\mathbf{G} = \begin{pmatrix} \mathbf{G}_1 & 0 \\ 0 & \mathbf{G}_2 \end{pmatrix}$ , are the

block-type diagonal matrices of thermodynamic forces and multiplier, respectively;

$$\mathbf{X}_{i} = \begin{pmatrix} X_{i} & 0 \\ 0 & X_{i} \end{pmatrix}, \quad \mathbf{G}_{i} = \begin{pmatrix} G_{i} & 0 \\ 0 & G_{i} \end{pmatrix},$$
$$\mathbf{\overline{V}} = \mathbf{GVG}^{-1} = \begin{pmatrix} \mathbf{V}_{11} & g_{12}\mathbf{V}_{12} \\ g_{21}\mathbf{V}_{21} & \mathbf{V}_{22} \end{pmatrix},$$

 $X_i = (\ln |G_i|)'_x$  is the thermodynamic force;  $G_1 = T^{-1}$ and  $G_2 = -\mu/T$  are the thermodynamic multipliers establishing the relationship between the changes in the physical properties and the entropy density;  $g_{ij} =$  $g_{ji}^{-1} = (G_i/G_j)$ ; *T* is the temperature; and  $\mu$  is the chemical potential of the diffusing component.

After perfoming the Fourier transform over x, we move to the equation for the vector function  $\hat{\mathbf{s}}(t, \varsigma)$ . Setting  $\zeta = 0$  and denoting  $\mathbf{S}(t) = \hat{\mathbf{s}}(t, 0)$ , we obtain the equation describing the process (8) in the entropy representation for the integral change in the vector function  $\mathbf{s}(t, x)$ :

$$d\mathbf{S}/dt = \sigma \mathbf{S},\tag{11}$$

where  $\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$  is the matrix operator of the

entropy source, which depends on the thermody-

namic forces 
$$X_i$$
;  $\mathbf{S} = \begin{pmatrix} \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix}$ ; and  $\mathbf{S}_i = \begin{pmatrix} S_1(t) \\ S_2(t) \end{pmatrix}$ ,  $i = 1, 2$ .

Here, the expressions for the block elements of the  $\sigma$  operator have the form  $\sigma_{ij} = (\Gamma_{ii} + X_i \mathbf{V}_{ij}), (i = j)$  and  $\sigma_{ij} = g_{ij} X_i \mathbf{V}_{ij}, (i \neq j)$ .

Since the heat and mass conservation laws must be satisfied independently, we impose the following conditions to extract the solutions satisfying Eqs. (8) and (11) from a set of mathematically feasible solutions:

They result in decomposing the equations into two  
two-component vector functions 
$$\mathbf{n}_i(t, x)$$
 and  $\mathbf{S}_i(t)$   
describing the superposition state of the system  $\langle \mathbf{n}_i |$  =

$$n_{1}^{(i)}\langle 1| + n_{2}^{(i)}\langle 2|, \langle \mathbf{S}_{i}| = S_{1}^{(i)}\langle 1| + S_{2}^{(i)}\langle 2|.$$
  

$$\frac{\partial \mathbf{n}_{i}}{\partial t} = \mathbf{H}_{i}\mathbf{n}_{i}, \qquad (13a)$$
  

$$\mathbf{n}_{i} = \begin{pmatrix} n_{1}^{(i)}(t, x) \\ n_{2}^{(i)}(t, x) \end{pmatrix},$$

$$\begin{aligned} \mathbf{H}_{i} &= \Gamma_{ii} \left( \begin{array}{c} -1 & 1 \\ 1 & -1 \end{array} \right) - \left( V_{0}^{(ii)} + V_{0}^{(ji)} \right) \left( \begin{array}{c} -1 & 0 \\ 0 & 1 \end{array} \right) \frac{\partial}{\partial x}, \\ &\frac{d\mathbf{S}_{i}}{dt} = \sigma_{i} \mathbf{S}_{i}, \end{aligned}$$
(13b)  
$$\mathbf{S}_{i} &= \left( \begin{array}{c} S_{1}^{(i)}(t) \\ S_{2}^{(i)}(t) \end{array} \right)_{i}, \\ &\sigma_{i} &= \Gamma_{ii} \left( \begin{array}{c} -1 & 1 \\ 1 & -1 \end{array} \right) + \left( X_{i} V_{0}^{(ii)} + g_{ji} X_{j} V_{0}^{(ji)} \right) \left( \begin{array}{c} -1 & 0 \\ 0 & 1 \end{array} \right), \end{aligned}$$

where  $nn_{1,2}^{(i)}(t, x)$  is the probability density of finding the system in states  $\langle 1|$  and  $\langle 2|$ ,  $S_{1,2}^{(i)}(t)$  is the integral change in the entropy in these states, and  $\sigma_i$  is the operator of the entropy source in the superposition state. Note that the probabilistic interpretation of the solution leads to the dimensions of the entropy source and the thermodynamic forces s<sup>-1</sup> and cm<sup>-1</sup>, respectively. This does not depend on process 1 or 2 and allows one to simplify the form of the resultant expressions.

Upon selecting the indices i = 1, j = 2, Eqs. (13) describe the heat transport under the action of the heat force  $X_1 = (\ln T^{-1})'_x$  and the heat process under action of the chemical force  $X_2 = (\ln |-\mu T^{-1}|)'_x$ , which was stimulated by the mass transport. Upon selecting the indices i = 2, j = 1, Eqs. (13) describe the mass transport under the action of the  $X_2$  force and the diffusion process under the action of the  $X_1$  force, which was stimulated by the heat transport.

According to [15], we consider that Eqs. (13) describe the transitions between states  $\langle 1|$  and  $\langle 2|$ . This brings two processes occurring on different time scales into correspondence. To describe these processes, we move to the stationary basis states  $\langle \mathbf{n}_{st}^i | = n_-^{(i)} \langle \mathbf{I} | + n_+^{(i)} \langle \mathbf{I} | |$ . After the canonical transformation  $\mathbf{H}_i = \mathbf{U}_n \mathbf{L}_i \mathbf{U}_n^{-1}$ ,  $\sigma_i = \mathbf{U}_s \mathbf{L}_i \mathbf{U}_s^{-1}$ and the denotation  $\mathbf{n}_{st}^{(i)} = \mathbf{U}_n^{-1} \mathbf{n}_i$ ,  $\mathbf{S}_{st}^{(i)} = \mathbf{U}_n^{-1} \mathbf{S}_i$ , we obtain

$$\frac{\partial \mathbf{n}_{st}^{(i)}}{\partial t} = \mathbf{L}_i \mathbf{n}_{st}^{(i)}, \qquad (14)$$

$$\mathbf{n}_{\mathrm{st}}^{(i)} = \begin{pmatrix} n_{-}(t,x) \\ n_{+}(t,x) \end{pmatrix}_{i}^{i}, \quad \mathbf{L}_{i} = \begin{pmatrix} \hat{L}_{-} & 0 \\ 0 & \hat{L}_{+} \end{pmatrix}^{i},$$
$$\hat{L}_{\mp}^{(i)} = -\Gamma_{ii} \left( 1 \mp \sqrt{1 + \left( (h_{i} + h_{ji}) \frac{\partial}{\partial x} \right)^{2}} \right),$$
$$h_{i} = \frac{V_{0}^{(i)}}{\Gamma_{ii}}, \quad h_{ji} = \frac{V_{0}^{(ji)}g_{ji}}{\Gamma_{ii}}, \quad (14a)$$

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$$\dot{\mathbf{S}}_{\mathrm{st}}^{(i)} = \Omega_i \mathbf{S}_{\mathrm{st}}^{(i)}, \qquad (15)$$

$$\mathbf{S}_{\text{st}}^{(i)} = \begin{pmatrix} S_{+}(t) \\ S_{-}(t) \end{pmatrix}_{i}, \quad \Omega_{i} = \begin{pmatrix} \Omega_{+} & 0 \\ 0 & \Omega_{-} \end{pmatrix},$$
$$\Omega_{\pm}^{(i)} = \Gamma_{ii}(-1 \pm \sqrt{1 + (h_{i}X_{i} + h_{ji}X_{i})^{2}}), \quad (15a)$$

where  $\mathbf{U}_{n,s}$  is the unitary operator;  $\Omega_i$  is the entropy

source operator in the stationary state; and  $\Omega_{\pm}^{(i)}$  are the expressions for the entropy source on the large and small time scales for the thermal i = 1 and diffusion i = 2 processes, respectively.

In Eqs. (12)–(14), the kinetic balance matrix  $G = G_{ii}$  provides the fulfillment of the conservation laws of the heat (mass)

$$\int_{-\infty}^{\infty} (n_1(t,x) + n_2(t,x))_i dx$$

$$= \int_{-\infty}^{\infty} n_-^{(i)}(t,x) dx = 1,$$
(16a)

and the entropy (for the system in the thermodynamic equilibrium state  $(X_i, X_j) = 0$ )

$$(S_{+}(t) + S_{-}(t))_{i} = S_{+}^{(i)}, \quad \dot{S}_{+}^{(i)} = 0,$$
 (16b)

in superposition states  $\langle 1|$  and  $\langle 2|$  and stationary state  $\langle I|.$ 

As in the case with the individual processes, the solutions  $n_{+}^{(i)}(t, x)$  and  $S_{-}^{(i)}(t)$  for stationary state  $\langle II|$  on the small time scale, the conservation laws for which are not fulfilled, do not take part in the conservation laws (16). Therefore, they are not observed in the experiment.

Because the processes in state  $\langle I |$  take place on the linear paths x = Vt,  $V \in [0, V_0^{(i)}]$ , where  $V_0^{(i)}$  is the limiting transport velocity, the question of the transition to the hydrodynamic scale with the paths in the form of  $o(\sqrt{t})$  arises. For this purpose, we restrict ourselves to the first terms of the expansion of the root in a series in (14a) and (15a) and describe the kinetics of the process for state  $\langle I |$  as follows:

$$\frac{\partial n_{-}^{(i)}}{\partial t} = (\hat{L}_{-}^{g} + ...) n_{-}^{(i)}, \quad \hat{L}_{-}^{g} = B_{i} \frac{\partial^{2}}{\partial x^{2}},$$

$$B_{i} = 0.5 \Gamma_{ii} (h_{i} + h_{ji})^{2}, \quad (17a)$$

$$\frac{dS_{+}^{(i)}}{dt} = (\Omega_{i}^{g} + ...) S_{+}^{(i)},$$

$$\Omega_i^g = B_{ii}X_i^2 + b_{ij}X_iX_j, \quad b_{ij} = \Gamma_{ii}h_{ii}h_{ji}, \quad (17b)$$

where all terms  $\hat{L}_{-}^{g}$  and  $\Omega_{i}^{g}$  give the hydrodynamic approximation of the transport processes, while the

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subsequent terms describe the influence of the inertia of the medium.

The difference between the coordinate and entropy representations are thus evident. Since the heat and mass conservation laws are fulfilled independently, the effect of the cross terms in (17a) is reduced only to the change (which is slight owing to the small cross effects) in the kinetic coefficients. Another case arises for representation (17b). The system entropy increases independently upon the occurrence of heat, diffusion, and cross processes. For the whole process, we finally obtain the well-known expression for the entropy source in the quadratic form of thermodynamic forces [16]:

$$\Omega_g = \Omega_1^g + \Omega_2^g = B_{11}X_1^2 + (b_{12} + b_{21})X_1X_2 + B_{22}X_2^2,$$
  
where  $b_{12} = b_{21}$ .

### CONCLUSIONS

1. A semiphenomenological model of the transport 2 processes under the action of intense energy sources making it possible to go outside the hydrodynamic approximation by considering the inertia of the medium on an external perturbation is proposed.

2. The model is based on the assumption of the possible existence of the system in both superposition and stationary basis states; in this case, the fluctuation and dissipative components of the processes are considered as a unified process wherein they are the components of the vector state.

3. It is shown that the observed deviations from a linear response of the medium to an external perturbation can be related to the inertia of the small-scale (fluctuation) processes.

4. It is also shown that, if the inertia of the medium is taken into account, the transport equations, which satisfy the conservation law, have the form of a system of first-order differential equations with two basis states.

5. Corrections to the classical equations and expressions for fluxes are found. They allow one to calculate the influence of the degree of nonequilibrium of the medium on the transport processes.

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SPELL: 1. quasiequilibrium, 2. semiphenomenological, 3. diffusivity, 4. Hamiltonian, 5. eatablishing

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