Statistical theory of catalytic hydrogen oxidation processes. Basic equations

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A statistical description for the processes of catalytic hydrogen oxidation is proposed taking into account the reaction–diffusion processes for magnetoactive ions and atoms adsorbed on the metal surface. The basic non-Markov transfer equations are obtained for the abbreviated description parameters of reaction-diffusion processes for magnetoactive ions and atoms adsorbed on the metal surface in the method of nonequilibrium statistical Zubarev operator. Weakly nonequilibrium reaction-diffusion processes are also considered.

1. Introduction

Environmental problems, which have recently become more acute and are largely associated with the negative impact of carbon monoxide (CO) on the one hand and significant interest in hydrogen energy on the other, pose the task of finding the latest efficient (nano-, sub-atomic) catalysts containing transition metals [1–17] for CO or H oxidation. Experimental development of such catalysts requires significant financial costs, but the predictability of their effective operation is quite limited.

The nature of surface phenomena in catalytic reactions is primarily due to the fact that the catalyst surface is magnetoactive (because of the electronic structure of the surface) in such reactions. Inhomogeneous magnetic fields created by magnetic spins of electrons localized on the surface of transition metals (Fe, Ni, Ru, Pt, Pd etc.) affect the processes of surface diffusion of particles (molecules, atoms, ions), which are magnetic dipoles on the surface. Of particular interest are the studies of diffusion and chemisorption processes for induced magnetic dipoles adsorbed on the surface of transition metals [6, 18–22], which are effective catalysts. They are relevant because the analysis of semi-phenomenological [23–27] and statistical models (the "lattice gas" models) [28] for description of CO oxidation kinetics shows that the surface quantum nature and interaction of CO, O_2 molecules and oxygen atoms with the catalyst surface both have a magneto-dipole nature and can cause the formation of CO clusters on the catalyst surface [29]. Even more interesting are the processes of hydrogen oxidation on the surface of metals, which are actively studied [30–34]. In particular, it is shown in [30] that the process of hydrogen oxidation is characterized by the presence of chemical current caused by the electron transfer [32, 33] and formation of bound states on the catalyst surface with electrons and reagents.

In this paper, a quantum-classical model is considered for describing the reaction-diffusion processes for magnetoactive ions and atoms adsorbed on the metal surface. A Hamiltonian of the model is constructed that takes into account the magneto-dipole nature of ions and atoms interaction and chemical catalytic bond with the surface of magnetoactive metal. In order to describe statistically and obtain reaction-diffusion equations, the main parameters of the abbreviated description are determined in the method of nonequilibrium statistical Zubarev operator [35–38].

2. Inhomogeneous transfer equations for description of reaction-diffusion processes for magnetoactive atoms adsorbed on the metal surface

The processes of dissociation and adsorption of O_2 on Pt are considered as the following successive processes. At $T \leqslant 45\,\text{K}$ there is "O_2" physical adsorption on the surface; in the temperature range of $90 - 135\,\text{K}$ O_2 molecule is converted into superoxide "O_2^-"; in the range of $135 - 150\,\text{K}$ it is converted into peroxide "O_2^{2-}", and then at higher temperatures to oxygen ion vapors "$O^- + O^-$". Schematically, these processes can be presented as follows:

$$O_2 + 2e^- \leftrightarrow \text{``}O_2 + 2e^-\text{''} \leftrightarrow \text{``}O_2^* + 2e^-\text{''} \leftrightarrow \text{``}O_2^{2-}\text{''} \leftrightarrow \text{``}2O^-\text{''}. \tag{1}$$
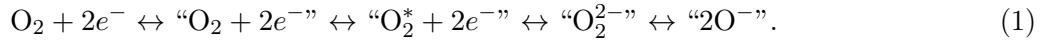
The process of hydrogen molecules adsorption is considered as formation of the bound state hydrogen atom-electron on the surface of platinum:

$$H_2 + 2e^- \Leftrightarrow \text{``}H_2 + 2e^-\text{''} \Leftrightarrow \text{``}2H^-\text{''}. \tag{2}$$
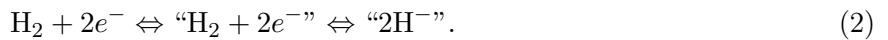
Then the oxidation process takes place first with formation of OH^- group and release of the electron

$$\text{``}O^- + H^-\text{''} \Leftrightarrow [\text{``}OH^- + e^-\text{''}]^{\neq} \Leftrightarrow \text{``}OH^- + e^-\text{''}, \tag{3}$$

and the next stage — formation of a water molecule and release of two electrons:

$$\text{``}OH^- + H^-\text{''} \Leftrightarrow [\text{``}OH^- + H + e^-\text{''}]^{\neq} \Leftrightarrow \text{``}H_2O^* + 2e^-\text{''}, \tag{4}$$
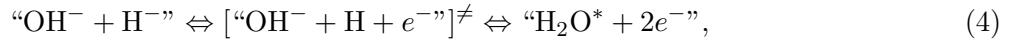
Here symbol $[\ldots]^{\neq}$ denotes the transition state and symbol "*" denotes the adsorbed state.

Anions of O^-, H^-, OH^- in adsorbed state on the platinum surface are magnetic dipoles in reactions (1)–(4) and H_2O^* is the dipole in adsorbed state. Therefore, from the point of view of model description, there is a system of magnetic dipole particles that fill the volume above the metal surface and can be adsorbed on it, interacting with the electron subsystem of metal surface.

For generality, we consider a system with $\bar{n}$ different sorts of magnetoactive particles (molecules, atoms, anions, electrons) with N_a number particles of sort a ($a = 1, \ldots, \bar{n}$). The Hamiltonian of the system is given as the sum of classical H_L and quantum $\hat{H}_q(t)$ parts:

$$\hat{H}(t) = H_L + \hat{H}_q(t), \tag{5}$$

where

$$H_L = \sum_a \sum_{j=1}^{N_a} \frac{p_j^2}{2m_a} + \frac{1}{2} \sum_{ab} \sum_{j \neq l} \Phi_{ab}(r_{jl}) + V_{ad}$$

is the classical part of Hamiltonian, which describes the system of magnetoactive particles as a simple classical gas, the atoms of sort a of which can be adsorbed on the magnetoactive surface of metal with an adsorption potential V_{ad}. r_{jl} is the distance between j and l particles, $\boldsymbol{p}_j$ and m_a are the vector momentum and the mass of magnetoactive particle of sort a, $\Phi_{ab}(r_{jl})$ is the pair potential of classical interaction between magnetoactive particles of sort a and b, which can be modeled by the Lennard–Jones potential. Values $a, b, \ldots$ in the sums are the indexes of the sort. An example of adsorption potential V_{ad} in the right part of the Hamiltonian is the Morse potential

$$V_{ad}(z) = D_e \left[1 - e^{C(z-z_e)}\right]^2,$$

where z is the coordinate in direction perpendicular to the surface, D_e is the depth of potential well for the equilibrium value of z_e coordinate, C is a constant. The quantum part of the Hamiltonian $\hat{H}_q(t)$

$$\hat{H}_q(t) = \hat{H}_e(t) + \hat{H}_S(t)$$

contains the contribution of electron subsystem:

$$\hat{H}_e(t) = \sum_{j=1}^{N_e} \frac{\left(\boldsymbol{p}_j - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r};t)\right)^2}{2m_e} + V_{ee},$$

with potential of electron-electron interaction V_{ee} (e is the electron charge, c is the speed of light, $\boldsymbol{A}(\boldsymbol{r};t)$ is the vector potential of electromagnetic field generated by electrons and magnetoactive particles in the system) and contribution $\hat{H}_S(t)$ describing a system of magnetoactive particles with spins $\boldsymbol{S}_j$ in the inhomogeneous magnetic field $\boldsymbol{B}'(\boldsymbol{r};t)$ and in the field created by N_m magnetoactive particles of the surface with coordinates $\boldsymbol{R}_f$ and spins, that can be presented as follows:

$$\hat{H}_S(t) = \hat{H}_S - \sum_a \int d\boldsymbol{r}\,\hat{\boldsymbol{M}}_a(\boldsymbol{r})\boldsymbol{B}_a(\boldsymbol{r};t). \tag{6}$$

Here $\boldsymbol{B}_a(\boldsymbol{r}_j;t) = \boldsymbol{B}'(\boldsymbol{r}_j;t) + \sum_{f=1}^{N_m} J_a(\boldsymbol{r}_j,\boldsymbol{R}_f)\boldsymbol{\sigma}_f$ is the total magnetic field acting on the j-th magnetic particle of sort a; $J_a(\boldsymbol{r}_j,\boldsymbol{R}_f)$ is the exchange integral for interaction of magnetoactive particles with magnetoactive sites of the metal surface, and

$$\hat{H}_S = -\frac{1}{2}\sum_{ab}\sum_{j\neq l} J_{ab}^{sh}(r_{jl})\boldsymbol{S}_j\boldsymbol{S}_l - \frac{1}{2}\sum_{ab}\sum_{\alpha\gamma}\sum_{j\neq l} J_{ab}^{l,\alpha\gamma}(r_{jl})S_j^\alpha S_l^\gamma$$
$$= -\sum_{ab}\frac{1}{2}\int d\boldsymbol{r}\int d\boldsymbol{r}'\, J_{ab}^{sh}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{S}_a(\boldsymbol{r})\boldsymbol{S}_b(\boldsymbol{r}') - \frac{1}{2}\sum_{ab}\sum_{\alpha\gamma}\int d\boldsymbol{r}\int d\boldsymbol{r} J_{ab}^{l,\alpha\gamma}(\boldsymbol{r},\boldsymbol{r}')S_a^\alpha(\boldsymbol{r})S_b^\gamma(\boldsymbol{r}')$$

is the quantum part of the Hamiltonian, which describes the system of magnetoactive particles; $\boldsymbol{S}_a(\boldsymbol{r}) = \sum_{j=1}^{N_a}\boldsymbol{S}_j\delta(\boldsymbol{r}-\boldsymbol{r}_j)$ is the spin $\boldsymbol{S}_j$ density operator of magnetic particles of sort a; $\hat{\boldsymbol{M}}_a(\boldsymbol{r}) = \mu_a\boldsymbol{S}_a(\boldsymbol{r})$ is the operator of magnetic moment density of magnetoactive particles of sort a. $J_{ab}(r_{jl})$ is the exchange integral for interaction of magnetoactive particles, which has two components: $J_{ab}^{sh}(r_{jl})$ is the short-term magnetic interaction, which can lead to a chemical bond between adsorbed particles of sort a and b, $J_{ab}^{l,\alpha\gamma}(r_{jl})$ are the components of tensor for long-range dipole-dipole interaction of adsorbed particles of sort a,b [22]:

$$J_{ab}^{l,\alpha\gamma}(r_{jl}) = -\frac{1}{2}(g_L\mu_B)^2\left(\frac{\delta_{\alpha\gamma}}{|\boldsymbol{r}_{jl}|^3} - \frac{3(\boldsymbol{r}_j-\boldsymbol{r}_l)^\alpha(\boldsymbol{r}_j-\boldsymbol{r}_l)^\gamma}{|\boldsymbol{r}_{jl}|^5}\right).$$

Here g_L is the Lang factor, μ_B is the Bohr magneton, $\alpha,\gamma = \{x,y,z\}$-components. Combining the exchange (Heisenberg) and dipole components, we introduce: $J_{ab}^{\alpha\beta}(\boldsymbol{r}) = J_{ab}^{sh}(r)\delta_{\alpha\gamma} + J_{ab}^{l,\alpha\gamma}(\boldsymbol{r})$ with $J_{ab}^{\alpha\gamma}(\boldsymbol{r})$ presented as the sum of diagonal and non-diagonal components:

$$J_{ab}^{\alpha\gamma}(\boldsymbol{r}) = J_{ab}^1(r)\delta_{\alpha\gamma} + J_{ab}^2(r)r^\alpha r^\gamma,$$

where

$$J_{ab}^1(r) = J_{ab}^{sh}(r) - \frac{1}{2}\frac{g_a g_b(\mu_B)^2}{r^3}, \quad J_{ab}^2(r) = \frac{3}{2}\frac{g_a g_b(\mu_B)^2}{r^5}$$

and g_a, g_b are the Lang factors of particles of sort a and b, respectively.

Hamiltonian $\hat{H}_S$ can now be written as

$$\hat{H}_S = -\frac{1}{2}\sum_{ab}\sum_{j\neq l} J_{ab}(r_{jl})\boldsymbol{S}_j\boldsymbol{S}_l$$
$$= -\frac{1}{2}\sum_{ab}\sum_{j\neq l} J_{ab}^1(r_{jl})(\boldsymbol{S}_j\cdot\boldsymbol{S}_l) - \frac{1}{2}\sum_{ab}\sum_{j\neq l} J_{ab}^2(r_{jl})(\boldsymbol{r}_{jl}\cdot\boldsymbol{S}_j)(\boldsymbol{r}_{jl}\cdot\boldsymbol{S}_l).$$

In order to describe the diffusional and magnetostrictive processes on the metal surface, we choose the average values of particle number density (molecules, atoms, anions, electrons) $\langle \hat{n}_a(\boldsymbol{r}) \rangle^t$ and magnetization $\langle \boldsymbol{M}_a(\boldsymbol{r}) \rangle^t$ as parameters (observed values) of the abbreviated description [39–41]. To study the cluster coverage and correlations, we also include the non-equilibrium structural functions "density – density" $\langle \hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$ and "spin–spin" $\langle \hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$ in the set of observed values, where $\langle \ldots \rangle^t = \mathrm{Sp}(\ldots \rho(t))$, $\rho(t)$ is the nonequilibrium statistical operator of a system. All dynamic variables and operators corresponding to the observed variables are defined as follows:

$$\hat{n}_a(\boldsymbol{r}) = \sum_{j=1}^{N_a} \delta(\boldsymbol{r} - \boldsymbol{r}_j)$$

is the microscopic density of number of magnetoactive particles of sort a,

$$\hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}') = \hat{n}_a(\boldsymbol{r}) \hat{n}_b(\boldsymbol{r}'),$$

$$\hat{G}_{ab}^{\alpha\gamma}(\boldsymbol{r}, \boldsymbol{r}') = S_a^\alpha(\boldsymbol{r}) S_b^\gamma(\boldsymbol{r}').$$

In order to obtain the transfer equations for parameters of the abbreviated description $\langle \hat{n}_a(\boldsymbol{r}) \rangle^t$, $\langle \boldsymbol{M}_a(\boldsymbol{r}) \rangle^t$, $\langle \hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$, $\langle \hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$, it is necessary to construct the corresponding nonequilibrium statistical operator $\rho(t)$, which satisfies the Liouville equation [35]. To obtain $\rho(t)$, we use the method of nonequilibrium statistical Zubarev operator [35, 36], taking into account the design procedure. In the general case, the nonequilibrium statistical operator can be represented as:

$$\rho(t) = \rho_q(t) - \int_{-\infty}^t e^{\varepsilon(t'-t)} \hat{T}(t, t') \big(1 - P_q(t')\big) i\hat{L}(t') \rho_q(t')\, dt', \tag{7}$$

where

$$\begin{aligned}
\rho_q(t) = \exp \Big\{ & -\Phi(t) - \beta\Big(\hat{H}(t) - \sum_a \int \mu_a(\boldsymbol{r}, t)\hat{n}_a(\boldsymbol{r})\, d\boldsymbol{r} \\
& - \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}'\, \overset{\leftrightarrow}{\mu}_{ba}(\boldsymbol{r}, \boldsymbol{r}'t) \bullet \hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \\
& - \sum_a \int d\boldsymbol{r}\, \hat{M}_a(\boldsymbol{r}) \cdot \boldsymbol{b}_a(\boldsymbol{r}; t) - \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}' \chi_{ba}(\boldsymbol{r}, \boldsymbol{r}'t)\hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}') - \mu_m N_m \Big) \Big\}
\end{aligned} \tag{8}$$

is the relevant statistical operator constructed from the extremum of information entropy of the system at fixed parameters of the abbreviated description $\langle \hat{n}_a(\boldsymbol{r}) \rangle^t$, $\langle \hat{\boldsymbol{M}}_a(\boldsymbol{r}) \rangle^t$, $\langle \hat{H}(t) \rangle^t$, $\langle \hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$, $\langle \hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$ and preserving a condition $\mathrm{Sp}\,\rho_q(t) = 1$, with $\langle \ldots \rangle^t = \mathrm{Sp}[\ldots \rho(t)]$, $\bullet$ denoting the tensor product. Here $\mu_a(\boldsymbol{r}, t)$ is the local chemical potential of magnetoactive particles of sort a, in the case of electrons $a = e$, $\mu_e(\boldsymbol{r}, t) = \bar{\mu}_e(\boldsymbol{r}, t) - e\varphi(\boldsymbol{r}, t)$ is the electrochemical potential, $\bar{\mu}_e(\boldsymbol{r}, t)$ is the local chemical potential of electrons, $\varphi(\boldsymbol{r}, t)$ is the scalar potential of electromagnetic field in the system. μ_m is the chemical potential of magnetoactive sites of the metal surface, $\beta = 1/k_{\mathrm{B}}T$ is the inverse temperature, k_{B} is the Boltzmann constant, $\boldsymbol{b}_a(\boldsymbol{r}; t)$ is the internal magnetic field created by magnetoactive particles of sort a, $\overset{\leftrightarrow}{\mu}_{ba}(\boldsymbol{r}, \boldsymbol{r}'t)$ are the Lagrange parameters and have a tensor dimension and are related to the correlation functions "spin density – spin density" $\langle \hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$, $\chi_{ba}(\boldsymbol{r}, \boldsymbol{r}'t)$ are the Lagrange parameters and play the role of chemical potential for complexes of $a\,b$ reagents and are conjugate to correlation functions "density – density" $\langle \hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \rangle^t$.

$$\begin{aligned}
\Phi(t) = \ln \mathrm{Sp} \exp \Big\{ & -\beta(t)\Big(\hat{H}(t) - \sum_a \int \mu_a(\boldsymbol{r}, t)\hat{n}_a(\boldsymbol{r})\, d\boldsymbol{r} - \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}'\, \overset{\leftrightarrow}{\mu}_{ba}(\boldsymbol{r}, \boldsymbol{r}'t) \bullet \hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}') \\
& - \sum_a \int d\boldsymbol{r}\, \hat{M}_a(\boldsymbol{r}) \cdot \boldsymbol{b}_a(\boldsymbol{r}; t) - \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}' \chi_{ba}(\boldsymbol{r}, \boldsymbol{r}'t)\hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}') - \mu_m N_m \Big) \Big\}
\end{aligned}$$

is the Masier–Planck functional. $i\hat{L}(t')$ is the Liouville operator corresponding to Hamiltonian (5) of the system, $P_q(t')$ is the Kawasaki–Ganton projection operator [36], the structure of which depends on the statistical operator (8), $\hat{T}(t,t') = \exp_+\{-\int_{t'}^{t}(1 - P_q(t''))i\hat{L}(t')dt''\}$ is the evolution operator based on the design. The Lagrange multipliers — nonequilibrium thermodynamic parameters $\mu_a(\boldsymbol{r},t)$, $\boldsymbol{b}_a(\boldsymbol{r};t)$, $\overset{\leftrightarrow}{\mu}_{ba}(\boldsymbol{r},\boldsymbol{r}'t)$, $\chi_{ba}(\boldsymbol{r},\boldsymbol{r}'t)$ are determined from the corresponding self-agreement conditions:

$$\langle\hat{n}_a(\boldsymbol{r})\rangle^t = \langle\hat{n}_a(\boldsymbol{r})\rangle_q^t, \quad \langle\hat{\boldsymbol{M}}_a(\boldsymbol{r})\rangle^t = \langle\hat{\boldsymbol{M}}_a(\boldsymbol{r})\rangle_q^t,$$
$$\langle\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t = \langle\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle_q^t, \quad \langle\hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t = \langle\hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle_q^t. \tag{9}$$

We substitute the relevant statistical operator into (7) and, performing the action of the Liouville operator on $\rho_q(t)$, we obtain for the nonequilibrium statistical operator:

$$\rho(t) = \rho_q(t) - \sum_a \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)}\hat{T}(t,t') \int_0^1 d\tau\, \rho_q^\tau(t')I_n^a(\boldsymbol{r}';t')\rho_q^{1-\tau}(t')\beta\mu_a(\boldsymbol{r}',t')\,dt'$$

$$- \sum_a \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)}\hat{T}(t,t') \int_0^1 d\tau\, \rho_q^\tau(t')I_M^a(\boldsymbol{r}';t')\rho_q^{1-\tau}(t')\beta\boldsymbol{b}_a(\boldsymbol{r}';t')\,dt'$$

$$- \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)}\hat{T}(t,t') \int_0^1 d\tau\, \rho_q^\tau(t')I_G^{ab}(\boldsymbol{r},\boldsymbol{r}';t')\rho_q^{1-\tau}(t')\beta\overset{\leftrightarrow}{\mu}_{ba}(\boldsymbol{r},\boldsymbol{r}'t')\,dt'$$

$$- \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)}\hat{T}(t,t') \int_0^1 d\tau\, \rho_q^\tau(t')I_g^{ab}(\boldsymbol{r},\boldsymbol{r}';t')\rho_q^{1-\tau}(t')\beta\chi_{ba}(\boldsymbol{r},\boldsymbol{r}'t')\,dt', \tag{10}$$

where

$$I_n^a(\boldsymbol{r}';t') = (1 - P(t'))i\hat{L}(t')\hat{n}_a(\boldsymbol{r}'), \quad I_M^a(\boldsymbol{r}';t') = (1 - P(t'))i\hat{L}(t')\hat{\boldsymbol{M}}_a(\boldsymbol{r}'), \tag{11}$$

$$I_G^{ab}(\boldsymbol{r},\boldsymbol{r}';t') = (1 - P(t'))i\hat{L}(t')\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}'), \quad I_g^{ab}(\boldsymbol{r},\boldsymbol{r}';t') = (1 - P(t'))i\hat{L}(t')\hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}') \tag{12}$$

are the microscopic generalized fluxes describing diffusion, magneto-diffusion and reaction processes in the system and on which there are built the generalized transfer coefficients and functions of reactions between components that describe, in particular, oxidation stages (1)–(4). $P(t')$ is the generalized Mori projection operator [35], which acts on dynamic variables (operators) and in this choice of abbreviated description parameters $\langle\hat{n}_a(\boldsymbol{r})\rangle^t$, $\langle\boldsymbol{M}_a(\boldsymbol{r})\rangle^t$, $\langle\hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t$, $\langle\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t$ has the following form:

$$P(t')A(\boldsymbol{r}) = \langle A(\boldsymbol{r})\rangle_q^t + \sum_a \int d\boldsymbol{r}' \frac{\delta\langle A(\boldsymbol{r})\rangle_q^t}{\delta\langle\hat{n}_a(\boldsymbol{r}')\rangle^t}\big(\hat{n}_a(\boldsymbol{r}') - \langle\hat{n}_a(\boldsymbol{r}')\rangle^t\big)$$

$$+ \sum_a \int d\boldsymbol{r}' \frac{\delta\langle A(\boldsymbol{r})\rangle_q^t}{\delta\langle\hat{\boldsymbol{M}}_a(\boldsymbol{r}')\rangle^t}\big(\hat{\boldsymbol{M}}_a(\boldsymbol{r}') - \langle\hat{\boldsymbol{M}}_a(\boldsymbol{r}')\rangle^t\big)$$

$$+ \sum_{ab} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \frac{\delta\langle A(\boldsymbol{r})\rangle_q^t}{\delta\langle\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r}',\boldsymbol{r}'')\rangle^t}\big(\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r}',\boldsymbol{r}'') - \langle\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r}',\boldsymbol{r}'')\rangle^t\big)$$

$$+ \sum_{ab} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \frac{\delta\langle A(\boldsymbol{r})\rangle_q^t}{\delta\langle\hat{g}_{ab}(\boldsymbol{r}',\boldsymbol{r}'')\rangle^t}\big(\hat{g}_{ab}(\boldsymbol{r}',\boldsymbol{r}'') - \langle\hat{g}_{ab}(\boldsymbol{r}',\boldsymbol{r}'')\rangle^t\big)$$

and the following properties $P(t)P(t') = P(t)$, $P(t)(1-P(t')) = 0$, $P(t)\hat{n}_a(\boldsymbol{r}') = \hat{n}_a(\boldsymbol{r}')$, $P(t)\hat{\boldsymbol{M}}_a(\boldsymbol{r}') = \hat{\boldsymbol{M}}_a(\boldsymbol{r}')$, $P(t)\overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r}',\boldsymbol{r}'') = \overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r}',\boldsymbol{r}'')$, $P(t)\hat{g}_{ab}(\boldsymbol{r}',\boldsymbol{r}'') = \hat{g}_{ab}(\boldsymbol{r}',\boldsymbol{r}'')$.

Using the nonequilibrium statistical operator $\rho(t)$ (10) one can obtain a system of transfer equations. To find the system of transfer equations, we use the fact that:

$$\frac{\partial}{\partial t}\langle\hat{X}\rangle^t = \langle\dot{\hat{X}}\rangle^t = \langle\dot{\hat{X}}\rangle_q^t + \langle(1 - P(t))\dot{\hat{X}}\rangle^t = \langle\dot{\hat{X}}\rangle_q^t + \langle I_X\rangle^t.$$

Using expression (10) for the nonequilibrium statistical operator, we obtain the transfer equation to describe the reaction-diffusion, magnetostrictive processes of magnetoactive particles that can be adsorbed on magnetoactive surface of the metal.

In expanded form, these transfer equations have the following structure:

$$\frac{\partial}{\partial t}\langle \hat{n}_a(\boldsymbol{r})\rangle^t = -\sum_b \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} \frac{\partial}{\partial \boldsymbol{r}} D_{nn}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t') \frac{\partial}{\partial \boldsymbol{r}'} \beta\mu_b(\boldsymbol{r}',t')\, dt'$$

$$-\sum_b \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} \frac{\partial}{\partial \boldsymbol{r}} D_{nR}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t') \frac{\partial}{\partial \boldsymbol{r}'} \beta\boldsymbol{b}_b(\boldsymbol{r}',t')\, dt'$$

$$-\sum_b \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} \frac{\partial}{\partial \boldsymbol{r}} D_{nM}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t') \beta\big(\boldsymbol{b}_b(\boldsymbol{r}',t') - \boldsymbol{B}(\boldsymbol{r}',t')\big)\, dt'$$

$$+\sum_{bc} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} \frac{\partial}{\partial \boldsymbol{r}} K_{nG}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \beta \overset{\leftrightarrow}{\mu}_{cb}(\boldsymbol{r}',\boldsymbol{r}'',t')\, dt'$$

$$+\sum_{bc} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} \frac{\partial}{\partial \boldsymbol{r}} K_{ng}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \beta\chi_{cb}(\boldsymbol{r}',\boldsymbol{r}'',t')\, dt'; \qquad (13)$$

$$\frac{\partial}{\partial t}\langle \hat{\boldsymbol{M}}_a(\boldsymbol{r})\rangle^t = \sum_b \int d\boldsymbol{r}' \Big\langle \frac{i}{h}[\hat{\boldsymbol{M}}_a(\boldsymbol{r}),\hat{\boldsymbol{M}}_b(\boldsymbol{r}')]\Big\rangle_q^t (\boldsymbol{b}_b(\boldsymbol{r}',t) - \boldsymbol{B}(\boldsymbol{r}',t))$$

$$-\sum_b \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} D_{Mn}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t') \frac{\partial}{\partial \boldsymbol{r}'} \beta\mu_b(\boldsymbol{r}',t')\, dt'$$

$$-\sum_b \int d\boldsymbol{r}' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} D_{MM}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t') \beta\big(\boldsymbol{b}_b(\boldsymbol{r}',t') - \boldsymbol{B}(\boldsymbol{r}',t')\big)\, dt'$$

$$-\sum_{bc} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} K_{MG}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \beta \overset{\leftrightarrow}{\mu}_{cb}(\boldsymbol{r}',\boldsymbol{r}'',t')\, dt'$$

$$-\sum_{bc} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} \frac{\partial}{\partial \boldsymbol{r}} K_{Mg}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \beta\chi_{cb}(\boldsymbol{r}',\boldsymbol{r}'',t')\, dt'; \qquad (14)$$

$$\frac{\partial}{\partial t}\langle \hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t = \Big\langle i\hat{L}(t)\hat{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}')\Big\rangle_q^t + \sum_c \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} K_{Gn}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \frac{\partial}{\partial \boldsymbol{r}''} \beta\mu_c(\boldsymbol{r}'',t')\, dt'$$

$$+\sum_c \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} K_{GR}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \frac{\partial}{\partial \boldsymbol{r}''} \beta\boldsymbol{b}_c(\boldsymbol{r}'',t')\, dt'$$

$$-\sum_c \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} K_{GM}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \beta\big(\boldsymbol{b}_c(\boldsymbol{r}'',t') - \boldsymbol{B}(\boldsymbol{r}'',t')\big)\, dt'$$

$$-\sum_{dc} \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} K_{GG}^{abcd}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''';t,t') \beta \overset{\leftrightarrow}{\mu}_{db}(\boldsymbol{r}'',\boldsymbol{r}''',t')\, dt'$$

$$-\sum_{dc} \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} K_{Gg}^{abcd}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''';t,t') \beta\chi_{dc}(\boldsymbol{r}'',\boldsymbol{r}''',t')\, dt'; \qquad (15)$$

$$\frac{\partial}{\partial t}\langle \hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t = \langle i\hat{L}(t')\hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle_q^t + \sum_c \int d\boldsymbol{r}'' \int_{-\infty}^{t} e^{\varepsilon(t'-t)} K_{gn}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t') \frac{\partial}{\partial \boldsymbol{r}''} \beta\mu_c(\boldsymbol{r}'',t')\, dt'$$

$$+ \sum_c \int d\boldsymbol{r}'' \int_{-\infty}^t e^{\varepsilon(t'-t)} K_{gR}^{abc}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}''; t, t') \frac{\partial}{\partial \boldsymbol{r}''} \beta \boldsymbol{b}_c(\boldsymbol{r}'', t') \, dt'$$

$$- \sum_c \int d\boldsymbol{r}'' \int_{-\infty}^t e^{\varepsilon(t'-t)} K_{gM}^{abc}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}''; t, t') \beta \big(\boldsymbol{b}_c(\boldsymbol{r}'', t') - \boldsymbol{B}(\boldsymbol{r}'', t') \big) \, dt'$$

$$- \sum_{dc} \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \int_{-\infty}^t e^{\varepsilon(t'-t)} K_{gG}^{abcd}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}'''; t, t') \beta \overset{\leftrightarrow}{\mu}_{db}(\boldsymbol{r}'', \boldsymbol{r}''', t') \, dt'$$

$$- \sum_{dc} \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \int_{-\infty}^t e^{\varepsilon(t'-t)} K_{gg}^{abcd}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}'''; t, t') \beta \chi_{dc}(\boldsymbol{r}'', \boldsymbol{r}''', t') \, dt'. \quad (16)$$

Here

$$D_{nn}^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t, t') = \mathrm{Sp}\left((1 - P(t)) \frac{1}{m_a} \hat{\boldsymbol{p}}_a(\boldsymbol{r}) T(t, t') \int_0^1 d\tau \rho_q^\tau(t')(1 - P(t')) \frac{1}{m_b} \hat{\boldsymbol{p}}_b(\boldsymbol{r}') \rho_q^{1-\tau}(t') \right)$$

is the generalized diffusion coefficient of magnetoactive particles, which is written in the form of Green–Kubo [35], $\hat{\boldsymbol{p}}_a(\boldsymbol{r}) = \sum_{j=1}^{N_a} \boldsymbol{p}_j \delta(\boldsymbol{r}' - \boldsymbol{r}_j)$ is the microscopic moment density of magnetoactive particles of sort a;

$$D_{nR}^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t, t') = \mathrm{Sp}\left((1 - P(t)) \frac{1}{m_a} \hat{\boldsymbol{p}}_a(\boldsymbol{r}) T(t, t') \int_0^1 d\tau \rho_q^\tau(t')(1 - P(t')) R_b(\boldsymbol{r}') \rho_q^{1-\tau}(t') \right)$$

is the generalized transfer coefficient describing magnetostrictive processes, where

$$R_b(\boldsymbol{r}') = \sum_{j=1}^{N_b} \frac{\boldsymbol{p}_j \mu_b \boldsymbol{S}_j}{m_b} \delta(\boldsymbol{r}' - \boldsymbol{r}_j).$$

$$D_{MM}^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t, t') = \mathrm{Sp}\left((1 - P(t)) i\hat{L}(t) \hat{\boldsymbol{S}}_a(\boldsymbol{r}) T(t, t') \int_0^1 d\tau \rho_q^\tau(t') \big(1 - P(t') \big) i\hat{L}(t) \hat{\boldsymbol{S}}_b(\boldsymbol{r}') \rho_q^{1-\tau}(t') \right)$$

is the generalized magnetic diffusion coefficient of magnetoactive particles of sort a and b. The generalized transfer coefficient $D_{Mn}^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t, t')$ as well as $D_{nR}^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t, t')$ describe the magnetostrictive processes. The generalized transfer kernels $K_{Gn}^{abc}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}''; t, t')$, $K_{GM}^{abc}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}''; t, t')$, $K_{GG}^{abcd}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}'''; t, t')$, $K_{Gg}^{abcd}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}''\boldsymbol{r}'''; t, t')$, $K_{gg}^{abcd}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}''\boldsymbol{r}'''; t, t')$ describe reaction-diffusion processes taking into account magnetic interaction and are correlation functions of the third and fourth order in terms of dynamic variables. In particular, function $K_{GG}^{abcd}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}'''; t, t')$ has the form:

$$K_{GG}^{abcd}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}'''; t, t') = \mathrm{Sp}\left((1 - P(t)) i\hat{L}(t) \overset{\leftrightarrow}{\hat{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}') T(t, t') \int_0^1 d\tau \, \rho_q^\tau(t') \right.$$
$$\left. \times (1 - P(t')) i\hat{L}(t) \overset{\leftrightarrow}{\hat{G}}_{cd}(\boldsymbol{r}'', \boldsymbol{r}''') \rho_q^{1-\tau}(t') \right). \quad (17)$$

The obtained here transfer coefficients and transfer kernels describe dissipative correlations in the system of magnetoactive particles (molecules, atoms, anions, electrons), which are in the inhomogeneous magnetic field of magnetoactive surface of the metal. They have a complex structure and describe the non-Markov, nonlinear diffusion, reaction-diffusion, magnetostrictive and spindiffusion processes. The influence of the magnetoactive surface on these processes is taken into account both through the magnetic field $\boldsymbol{B}(\boldsymbol{r}; t)$ and through the magnetic interaction and adsorption potential included in the Hamiltonian of the system. The obtained transfer equations (13)-(16) can describe diffusion, magnetostrictive and spindiffusion processes also in the presence of external magnetic fields.

3. Reaction–diffusion transfer equations for weakly nonequilibrium catalytic processes

We consider the reaction-diffusion processes characterized by small fluctuations of nonequilibrium thermodynamic parameters $\boldsymbol{F}_\nu(\boldsymbol{r};t)$ and $\boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}';t)$

$$\boldsymbol{F}_\nu(\boldsymbol{r};t) = (\beta\mu_a(\boldsymbol{r};t), \beta\boldsymbol{b}_a(\boldsymbol{r};t))^{\mathrm{T}},$$

$$\boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}';t) = (\beta\overset{\leftrightarrow}{\mu}_{ab}(\boldsymbol{r},\boldsymbol{r}';t), \beta\chi_{ab}(\boldsymbol{r},\boldsymbol{r}';t))^{\mathrm{T}}.$$

from their locally equilibrium values $\boldsymbol{F}_\nu(\boldsymbol{r})$ and $\boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}')$. In this case, we decompose the relevant statistical operator $\rho_q(t)$ by fluctuations $\delta\boldsymbol{F}_\nu(\boldsymbol{r};t) = \boldsymbol{F}_\nu(\boldsymbol{r};t) - \boldsymbol{F}_\nu(\boldsymbol{r})$ and $\delta\boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}';t) = \boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}';t) - \boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}')$ into a series and limit ourselves to a linear approximation by these fluctuations. In this approximation, the fluctuations of nonequilibrium thermodynamic parameters $\delta\boldsymbol{F}_\nu(\boldsymbol{r};t)$, $\delta\boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}';t)$ are determined from the corresponding self-agreement conditions (9). As a result, for the relevant statistical operator we obtain in this approximation:

$$
\begin{aligned}
\rho_q^0(t) = \rho_0 \bigg(& 1 + \sum_{ab} \iint \langle\delta\hat{n}_a(\boldsymbol{r})\rangle^t [\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r},\boldsymbol{r}')]_{ab} \hat{n}_b(\boldsymbol{r}';\tau)\, d\boldsymbol{r}\, d\boldsymbol{r}' \\
& + \sum_{ab} \iint \langle\delta\bar{\boldsymbol{M}}_a(\boldsymbol{r})\rangle^t [\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r},\boldsymbol{r}')]_{ab} \bar{\boldsymbol{M}}_b(\boldsymbol{r}';\tau)\, d\boldsymbol{r}\, d\boldsymbol{r}' \\
& + \sum_{abcd} \iiiint \langle\delta\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t [\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r},\boldsymbol{r}';\boldsymbol{r}'',\boldsymbol{r}''')]_{abcd} \bar{g}_{cd}(\boldsymbol{r}'',\boldsymbol{r}''';\tau)\, d\boldsymbol{r}\, d\boldsymbol{r}'\, d\boldsymbol{r}''\, d\boldsymbol{r}''' \\
& + \sum_{abcd} \iiiint \langle\delta\overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^t [\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r},\boldsymbol{r}';\boldsymbol{r}'',\boldsymbol{r}''')]_{abcd} \overset{\leftrightarrow}{G}_{cd}(\boldsymbol{r}'',\boldsymbol{r}''';\tau)\, d\boldsymbol{r}\, d\boldsymbol{r}'\, d\boldsymbol{r}''\, d\boldsymbol{r}''' \bigg),
\end{aligned} \qquad (18)
$$

where

$$
\begin{aligned}
\rho_0 = \exp\bigg\{ & -\Phi - \beta\Big(\hat{H} - \sum_a \int \mu_a(\boldsymbol{r})\hat{n}_a(\boldsymbol{r})d\boldsymbol{r} - \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}' \overset{\leftrightarrow}{\mu}_{ba}(\boldsymbol{r},\boldsymbol{r})\overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}') \\
& - \sum_a \int d\boldsymbol{r}\hat{\boldsymbol{M}}_a(\boldsymbol{r})\boldsymbol{b}_a(\boldsymbol{r}) - \sum_{ab} \int d\boldsymbol{r} \int d\boldsymbol{r}'\chi_{ba}(\boldsymbol{r},\boldsymbol{r}')\hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}') - \mu_m N_m \bigg\}
\end{aligned} \qquad (19)
$$

is the equilibrium statistical operator of the system. $A(\boldsymbol{r};\tau) = \int_0^1 d\tau\rho_0^\tau A(\boldsymbol{r})\rho_0^{-\tau}$. In this approximation, the fluctuations of parameters in the abbreviated description of nonequilibrium processes have the following structure: $\delta\hat{n}_a(\boldsymbol{r}) = \hat{n}_a(\boldsymbol{r}) - \langle\hat{n}_a(\boldsymbol{r})\rangle_0$, $\delta\bar{\boldsymbol{M}}_a(\boldsymbol{r}) = \bar{\boldsymbol{M}}_a(\boldsymbol{r}) - \langle\bar{\boldsymbol{M}}_a(\boldsymbol{r})\rangle_0$, $\delta\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}') = \bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}') - \langle\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle_0$, $\delta\overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}') = \overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}') - \langle\overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle_0$, ($\langle\ldots\rangle_0 = \mathrm{Sp}[\ldots\rho_0]$ is the averaging with the equilibrium statistical operator ρ_0) in which $\bar{\boldsymbol{M}}_a(\boldsymbol{r})$, $\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')$, $\overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}')$ are the new description parameters, that arose by excluding nonequilibrium parameters $\delta\boldsymbol{F}_\nu(\boldsymbol{r};t)$, $\delta\boldsymbol{F}_\eta(\boldsymbol{r},\boldsymbol{r}';t)$ from the corresponding self-agreement conditions (9):

$$\bar{\boldsymbol{M}}_a(\boldsymbol{r}) = (1 - P_{nn})\hat{\boldsymbol{M}}_a(\boldsymbol{r}), \qquad (20)$$

where P_{nn} is the Mori–type projection operator built on variables $\hat{n}_b(\boldsymbol{r}')$

$$P_{nn}(\ldots) = \sum_{bc} \iint \langle\ldots\hat{n}_b(\boldsymbol{r}')\rangle_0 [\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')]_{bc}\hat{n}_c(\boldsymbol{r}'';\tau)\, d\boldsymbol{r}'\, d\boldsymbol{r}'', \qquad (21)$$

$$\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}') = (1 - P_{nn} - P_{\bar{M}\bar{M}})\hat{g}_{ab}(\boldsymbol{r},\boldsymbol{r}'), \qquad (22)$$

and $P_{\bar{M}\bar{M}}$ is the Mori–type projection operator built on variables $\bar{\boldsymbol{M}}_c(\boldsymbol{r}'')$

$$P_{\bar{M}\bar{M}}(\ldots) = -\sum_{cd} \iint \langle\ldots\bar{\boldsymbol{M}}_c(\boldsymbol{r}'')\rangle_0 [\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')]_{cd}\bar{\boldsymbol{M}}_d(\boldsymbol{r}''';\tau)\, d\boldsymbol{r}''\, d\boldsymbol{r}''', \qquad (23)$$

$$\overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}') = (1 - P_{nn} - P_{\bar{M}\bar{M}} - P_{\bar{g}\bar{g}})\overset{\leftrightarrow}{G}_{ab}(\boldsymbol{r},\boldsymbol{r}'), \qquad (24)$$

and $P_{\bar{g}\bar{g}}$ is the Mori–type projection operator built on variables $\bar{g}_{cd}(\boldsymbol{r}'', \boldsymbol{r}''')$

$$P_{\bar{g}\bar{g}}(\dots) = \sum_{cdc'd'} \iiiint \langle \dots \bar{g}_{cd}(\boldsymbol{r}'', \boldsymbol{r}''')\rangle_0 \big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}'', \boldsymbol{r}'''; \boldsymbol{r}'''', \boldsymbol{r}''''')\big]_{cdc'd'} \bar{g}_{c'd'}(\boldsymbol{r}'''', \boldsymbol{r}'''''; \tau) d\boldsymbol{r}'' d\boldsymbol{r}''' d\boldsymbol{r}'''' d\boldsymbol{r}'''''.$$
(25)

In the structure of projection operators P_{nn}, $P_{\bar{M}\bar{M}}$, $P_{\bar{g}\bar{g}}$ the corresponding functions $[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')]_{bc}$ are the elements of matrix inverse to the matrix, elements of which are $\Phi_{nn}^{ca}(\boldsymbol{r}'', \boldsymbol{r}) = \langle \hat{n}_c(\boldsymbol{r}'')\hat{n}_a(\boldsymbol{r}; \tau)\rangle_0 = \langle \hat{g}_{ca}(\boldsymbol{r}'', \boldsymbol{r})\rangle_0$ — the equilibrium pair structural distribution functions of the corresponding particles. Functions $[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')]_{bc}$ are found from integral relations

$$\sum_c \int \big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{bc} \Phi_{nn}^{ca}(\boldsymbol{r}'', \boldsymbol{r})\, d\boldsymbol{r}'' = \delta_{ba}\delta(\boldsymbol{r}' - \boldsymbol{r}).$$
(26)

Functions $\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{bc}$ are the elements of matrix inverse to the matrix, elements of which are $\Phi_{\bar{M}\bar{M}}^{ca}(\boldsymbol{r}'', \boldsymbol{r})$ — the equilibrium correlation functions that describe the magnetic, magnetostrictive and structural properties of particles in the system. $\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{bc}$ are found from integral relations

$$\sum_c \int \big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{bc} \Phi_{\bar{M}\bar{M}}^{ca}(\boldsymbol{r}'', \boldsymbol{r}) d\boldsymbol{r}'' = \delta_{ba}\delta(\boldsymbol{r}' - \boldsymbol{r}),$$
(27)

with the correlation function $\Phi_{\bar{M}\bar{M}}^{ca}(\boldsymbol{r}'', \boldsymbol{r})$ in the following form:

$$\begin{aligned}
\Phi_{\bar{M}\bar{M}}^{ca}(\boldsymbol{r}'', \boldsymbol{r}) &= \big\langle (1 - P_{nn})\hat{\boldsymbol{M}}_c(\boldsymbol{r}'')(1 - P_{nn})\hat{\boldsymbol{M}}_a(\boldsymbol{r}; \tau)\big\rangle_0 \\
&= \Phi_{MM}^{ca}(\boldsymbol{r}'', \boldsymbol{r}) - \sum_{b'c'} \iint \Phi_{Mn}^{cb'}(\boldsymbol{r}'', \boldsymbol{r}''')\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}''', \boldsymbol{r}'''')\big]_{b'c'} \Phi_{nM}^{c'a}(\boldsymbol{r}'''', \boldsymbol{r}) d\boldsymbol{r}''' d\boldsymbol{r}'''' \\
&\quad - \sum_{d'k'} \iint \Phi_{Mn}^{ad'}(\boldsymbol{r}, \boldsymbol{r}''''')\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}''''', \boldsymbol{r}'''''')\big]_{d'k'} \Phi_{nM}^{k'c}(\boldsymbol{r}'''''', \boldsymbol{r}'') d\boldsymbol{r}''''' d\boldsymbol{r}'''''' \\
&\quad - \sum_{b'c'd'k'} \iiiint \Phi_{Mn}^{cb'}(\boldsymbol{r}'', \boldsymbol{r}''')\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}''', \boldsymbol{r}'''')\big]_{b'c'} \Phi_{Mn}^{ad'}(\boldsymbol{r}, \boldsymbol{r}''''') \\
&\quad \times \big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}''''', \boldsymbol{r}'''''')\big]_{d'k'} \Phi_{nn}^{c'k'}(\boldsymbol{r}'''''', \boldsymbol{r}'''') d\boldsymbol{r}''' d\boldsymbol{r}'''' d\boldsymbol{r}''''' d\boldsymbol{r}'''''',
\end{aligned}$$
(28)

where $\Phi_{MM}^{ca}(\boldsymbol{r}'', \boldsymbol{r})$ is the equilibrium correlation function "density of magnetic moment – density of magnetic moment" of particles of sort c, a, $\Phi_{Mn}^{cb'}(\boldsymbol{r}'', \boldsymbol{r}''')$ are the equilibrium correlation functions describing the magnetostrictive properties in the system. Functions $\big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''', \boldsymbol{r}'''')\big]_{bcc'd'}$, $\big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''', \boldsymbol{r}'''')\big]_{bcc'd'}$ are found from the corresponding integral relations

$$\sum_{c'd'} \iint \big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''', \boldsymbol{r}'''')\big]_{bcc'd'} \Phi_{\bar{g}\bar{g}}^{c'd'ad}(\boldsymbol{r}''', \boldsymbol{r}''''; \boldsymbol{r}, \boldsymbol{r}''''') d\boldsymbol{r}''' d\boldsymbol{r}'''' = \delta_{bc}\delta_{ad}\delta(\boldsymbol{r}' - \boldsymbol{r})\delta(\boldsymbol{r}'' - \boldsymbol{r}'''''), \quad (29)$$

$$\sum_{c'd'} \iint \big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''', \boldsymbol{r}'''')\big]_{bcc'd'} \Phi_{\bar{G}\bar{G}}^{c'd'ad}(\boldsymbol{r}''', \boldsymbol{r}''''; \boldsymbol{r}, \boldsymbol{r}''''') d\boldsymbol{r}''' d\boldsymbol{r}'''' = \delta_{bc}\delta_{ad}\delta(\boldsymbol{r}' - \boldsymbol{r})\delta(\boldsymbol{r}'' - \boldsymbol{r}''''') \quad (30)$$

under condition of calculating the fourth order correlation functions $\Phi_{\bar{g}\bar{g}}^{c'd'ad}(\boldsymbol{r}''', \boldsymbol{r}''''; \boldsymbol{r}, \boldsymbol{r}''''')$ $\Phi_{\bar{G}\bar{G}}^{c'd'ad}(\boldsymbol{r}''', \boldsymbol{r}''''; \boldsymbol{r}, \boldsymbol{r}''''')$ on variables of particle number density $\hat{n}_a(\boldsymbol{r})$ and magnetic moment density $\hat{\boldsymbol{M}}_a(\boldsymbol{r})$, which have the following structure:

$$\Phi_{\bar{g}\bar{g}}^{c'd'ad}(\boldsymbol{r}''', \boldsymbol{r}''''; \boldsymbol{r}, \boldsymbol{r}''''') = \Big\langle (1 - P_{nn} - P_{\bar{M}\bar{M}})\hat{g}_{c'd'}(\boldsymbol{r}''', \boldsymbol{r}'''')(1 - P_{nn} - P_{\bar{M}\bar{M}})\hat{g}_{ad}(\boldsymbol{r}, \boldsymbol{r}'''''; \tau)\Big\rangle_0, \quad (31)$$

$$\Phi_{\bar{G}\bar{G}}^{c'd'ad}(\boldsymbol{r}''', \boldsymbol{r}''''; \boldsymbol{r}, \boldsymbol{r}''''') = \Big\langle (1 - P_{nn} - P_{\bar{M}\bar{M}} - P_{\bar{g}\bar{g}})\hat{\overset{\leftrightarrow}{G}}_{c'd'}(\boldsymbol{r}''', \boldsymbol{r}'''')(1 - P_{nn} - P_{\bar{M}\bar{M}} - P_{\bar{g}\bar{g}})\hat{\overset{\leftrightarrow}{G}}_{ad}(\boldsymbol{r}, \boldsymbol{r}'''''; \tau)\Big\rangle_0.$$

It is important to note that in this linear approximation the dynamic variables $\hat{n}_a(\boldsymbol{r})$ $\bar{\boldsymbol{M}}_a(\boldsymbol{r})$, $\bar{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}')$, $\overleftrightarrow{\bar{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}')$ are orthogonal in the sense of mean values:

$$\langle \hat{n}_a(\boldsymbol{r})\bar{\boldsymbol{M}}_b(\boldsymbol{r}'; \tau)\rangle_0 = 0, \quad \langle \hat{n}_a(\boldsymbol{r})\bar{g}_{cb}(\boldsymbol{r}', \boldsymbol{r}''; \tau)\rangle_0 = 0, \quad \left\langle \hat{n}_a(\boldsymbol{r})\overleftrightarrow{\bar{G}}_{cb}(\boldsymbol{r}', \boldsymbol{r}''; \tau)\right\rangle_0 = 0,$$

$$\langle \bar{\boldsymbol{M}}_a(\boldsymbol{r})\bar{g}_{cb}(\boldsymbol{r}', \boldsymbol{r}''; \tau)\rangle_0 = 0, \quad \left\langle \bar{\boldsymbol{M}}_a(\boldsymbol{r})\overleftrightarrow{\bar{G}}_{cb}(\boldsymbol{r}', \boldsymbol{r}''; \tau)\right\rangle_0 = 0, \quad \left\langle \bar{g}_{ad}(\boldsymbol{r}', \boldsymbol{r}'')\overleftrightarrow{\bar{G}}_{cb}(\boldsymbol{r}''', \boldsymbol{r}''''; \tau)\right\rangle_0 = 0.$$

Since, expression for the relevant statistical operator is obtained in the linear approximation for fluctuations of the nonequilibrium thermodynamic parameters, we can construct a nonequilibrium statistical operator in this approximation. Substituting (19) into (7) after simple transformations, we obtain:

$$\rho(t) = \rho_q^0(t) - \sum_{ab} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int_{-\infty}^t e^{\varepsilon(t'-t)} \hat{T}_0(t, t') \int_0^1 d\tau (\rho_0^\tau I_n^a(\boldsymbol{r}'; t')\rho_0^{1-\tau}) \big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{ab} \langle \delta\hat{n}_b(\boldsymbol{r}'')\rangle^{t'} dt'$$

$$- \sum_{ab} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int_{-\infty}^t e^{\varepsilon(t'-t)} \hat{T}_0(t, t') \int_0^1 d\tau (\rho_0^\tau I_M^a(\boldsymbol{r}'; t')\rho_0^{1-\tau}) \big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{ab} \langle \delta\bar{\boldsymbol{M}}_b(\boldsymbol{r}'')\rangle^{t'} dt'$$

$$- \sum_{abcd} \int d\boldsymbol{r} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \int_{-\infty}^t e^{\varepsilon(t'-t)} \hat{T}_0(t, t') \int_0^1 d\tau (\rho_0^\tau I_G^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t')\rho_0^{1-\tau})$$

$$\times \big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''')\big]_{abcd} \langle \delta\overleftrightarrow{\bar{G}}_{cd}(\boldsymbol{r}'', \boldsymbol{r}''')\rangle^{t'} dt'$$

$$- \sum_{abcd} \int d\boldsymbol{r} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \int_{-\infty}^t e^{\varepsilon(t'-t)} \hat{T}_0(t, t') \int_0^1 d\tau (\rho_0^\tau I_g^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t')\rho_0^{1-\tau})$$

$$\times \big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''')\big]_{abcd} \langle \delta\bar{g}_{cd}(\boldsymbol{r}'', \boldsymbol{r}''')\rangle^{t'} dt', \tag{32}$$

where

$$I_n^a(\boldsymbol{r}'t') = (1 - P)i\hat{L}(t')\hat{n}_a(\boldsymbol{r}'), \quad I_M^a(\boldsymbol{r}'; t') = (1 - P)i\hat{L}(t')\hat{\boldsymbol{M}}_a(\boldsymbol{r}'), \tag{33}$$

$$I_G^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t') = (1 - P)i\hat{L}(t')\overleftrightarrow{\hat{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}'), \quad I_g^{ab}(\boldsymbol{r}, \boldsymbol{r}'; t') = (1 - P)i\hat{L}(t')\hat{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}')$$

are the microscopic generalized fluxes describing diffusion, magneto-diffusion and reaction weakly nonequilibrium processes in the system and on which the generalized transfer coefficients and functions of reactions between components are built. P is the generalized Mori projection operator in the linear approximation by fluctuations and has the following structure:

$$P(\ldots) = \sum_{ab} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \langle \ldots \hat{n}_a(\boldsymbol{r}'; \tau)\rangle_0 \big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{ab} \hat{n}_b(\boldsymbol{r}'')$$

$$+ \sum_{ab} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \langle \ldots \bar{\boldsymbol{M}}_a(\boldsymbol{r}'; \tau)\rangle_0 \big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}', \boldsymbol{r}'')\big]_{ab} \bar{\boldsymbol{M}}_b(\boldsymbol{r}'')$$

$$+ \sum_{abcd} \int d\boldsymbol{r} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \left\langle \ldots \overleftrightarrow{\bar{G}}_{ab}(\boldsymbol{r}, \boldsymbol{r}'; \tau)\right\rangle_0 \big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''')\big]_{abcd} \overleftrightarrow{\bar{G}}_{cd}(\boldsymbol{r}'', \boldsymbol{r}''')$$

$$+ \sum_{abcd} \int d\boldsymbol{r} \int d\boldsymbol{r}' \int d\boldsymbol{r}'' \int d\boldsymbol{r}''' \langle \ldots \bar{g}_{ab}(\boldsymbol{r}, \boldsymbol{r}'; \tau)\rangle_0 \big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'', \boldsymbol{r}''')\big]_{abcd} \bar{g}_{cd}(\boldsymbol{r}'', \boldsymbol{r}''').$$

$\hat{T}_0(t, t')$ is the evolution operator taking into account the design procedure in the linear approximation by fluctuations. The time dependence of the generalized fluxes (33) is related to the action of the Liouville operator $i\hat{L}(t')$, which corresponds to the Hamiltonian of the system (5) that contains an external time-dependent magnetic field. By structure, the nonequilibrium statistical operator (32) is a linear functional by fluctuations of the abbreviated description parameters $\langle \delta\hat{n}_b(\boldsymbol{r}'')\rangle^{t'}$, $\langle \delta\bar{\boldsymbol{M}}_b(\boldsymbol{r}'')\rangle^{t'}$,

$\langle\delta\bar{\overset{\leftrightarrow}{G}}_{cd}(\boldsymbol{r}'',\boldsymbol{r}''')\rangle^{t'}$, $\langle\delta\bar{g}_{cd}(\boldsymbol{r}'',\boldsymbol{r}''')\rangle^{t'}$. With the help of it, we obtain a closed system of non-Markov in time integro-differential equations for fluctuations of the abbreviated description parameters:

$$\frac{\partial}{\partial t}\langle\delta\hat{n}_a(\boldsymbol{r})\rangle^t = -\sum_b\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int_{-\infty}^t e^{\varepsilon(t'-t)}\frac{\partial}{\partial\boldsymbol{r}}\bar{D}_{nn}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t')\frac{\partial}{\partial\boldsymbol{r}'}\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')\big]_{bc}\langle\delta\hat{n}_c(\boldsymbol{r}'')\rangle^{t'}dt'$$

$$+\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int_{-\infty}^t e^{\varepsilon(t'-t)}\frac{\partial}{\partial\boldsymbol{r}}\bar{D}_{nR}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t')\frac{\partial}{\partial\boldsymbol{r}'}\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')\big]_{bc}\langle\delta\bar{\boldsymbol{M}}_c(\boldsymbol{r}'')\rangle^{t'}dt'$$

$$+\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int_{-\infty}^t e^{\varepsilon(t'-t)}\frac{\partial}{\partial\boldsymbol{r}}\bar{D}_{nM}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t')\big(\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')\big]_{bc}\langle\delta\bar{\boldsymbol{M}}_c(\boldsymbol{r}'')\rangle^{t'}+\beta\boldsymbol{B}(\boldsymbol{r}',t')\big)dt'$$

$$-\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int_{-\infty}^t e^{\varepsilon(t'-t)}\frac{\partial}{\partial\boldsymbol{r}}\bar{K}_{nG}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''')\big]_{bcdc'}\langle\delta\bar{\overset{\leftrightarrow}{G}}_{dc'}(\boldsymbol{r}''',\boldsymbol{r}'''')\rangle^{t'}dt'$$

$$-\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int_{-\infty}^t e^{\varepsilon(t'-t)}\frac{\partial}{\partial\boldsymbol{r}}\bar{K}_{ng}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''')\big]_{bcdc'}\langle\delta\bar{g}_{dc'}(\boldsymbol{r}''',\boldsymbol{r}'''')\rangle^{t'}dt', \tag{34}$$

$$\frac{\partial}{\partial t}\langle\delta\hat{\boldsymbol{M}}_a(\boldsymbol{r})\rangle^t = -\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\Big\langle\frac{i}{h}[\hat{\boldsymbol{M}}_a(\boldsymbol{r}),\hat{\boldsymbol{M}}_b(\boldsymbol{r}')]\Big\rangle_0^t\big(\beta^{-1}\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')\big]_{bc}\langle\delta\bar{\boldsymbol{M}}_c(\boldsymbol{r}'')\rangle^t+\boldsymbol{B}(\boldsymbol{r}',t)\big)$$

$$+\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{D}_{Mn}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t')\frac{\partial}{\partial\boldsymbol{r}'}\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')\big]_{bc}\langle\delta\hat{n}_c(\boldsymbol{r}'')\rangle^{t'}dt'$$

$$+\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{D}_{MM}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t')\big(\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')\big]_{bc}\langle\delta\bar{\boldsymbol{M}}_c(\boldsymbol{r}'')\rangle^{t'}+\beta\boldsymbol{B}(\boldsymbol{r}',t')\big)dt'$$

$$+\sum_{bcdc'}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{K}_{MG}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''')\big]_{bcdc'}\Big\langle\delta\bar{\overset{\leftrightarrow}{G}}_{dc'}(\boldsymbol{r}''',\boldsymbol{r}'''')\Big\rangle^{t'}dt'$$

$$+\sum_{bcdc'}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{K}_{Mg}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''')\big]_{bcdc'}\langle\delta\bar{g}_{dc'}(\boldsymbol{r}''',\boldsymbol{r}'''')\rangle^{t'}dt', \tag{35}$$

$$\frac{\partial}{\partial t}\Big\langle\delta\bar{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}')\Big\rangle^t = \Big\langle i\hat{L}(t')\delta\bar{\overset{\leftrightarrow}{G}}_{ab}(\boldsymbol{r},\boldsymbol{r}')\Big\rangle_{q0}^t$$

$$-\sum_{cd}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{K}_{Gn}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')\frac{\partial}{\partial\boldsymbol{r}''}\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')\big]_{cd}\langle\delta\hat{n}_d(\boldsymbol{r}''')\rangle^{t'}dt'$$

$$+\sum_{cd}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{K}_{GR}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')\frac{\partial}{\partial\boldsymbol{r}''}\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')\big]_{cd}\langle\delta\bar{\boldsymbol{M}}_d(\boldsymbol{r}''')\rangle^{t'}dt'$$

$$+\sum_{cd}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{K}_{GM}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')\big(\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')\big]_{cd}\langle\delta\bar{\boldsymbol{M}}_d(\boldsymbol{r}''')\rangle^{t'}+\beta\boldsymbol{B}(\boldsymbol{r}',t')\big)dt'$$

$$+\sum_{dcc'd'}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int d\boldsymbol{r}'''''\int_{-\infty}^t e^{\varepsilon(t'-t)}\bar{K}_{GG}^{abcd}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''';t,t')$$

$$\times \big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''',\boldsymbol{r}''''')\big]_{cdc'd'}\langle\delta\overset{\overleftrightarrow{}}{\bar{G}}_{c'd'}(\boldsymbol{r}'''',\boldsymbol{r}''''')\rangle^{t'}dt'$$

$$+\sum_{dcc'd'}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int d\boldsymbol{r}'''''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{Gg}^{abcd}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}''\boldsymbol{r}''';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''',\boldsymbol{r}''''')\big]_{cdc'd'}\langle\delta\bar{g}_{c'd'}(\boldsymbol{r}'''',\boldsymbol{r}''''')\rangle^{t'}dt', \tag{36}$$

$$\frac{\partial}{\partial t}\langle\delta\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^{t}=\langle i\hat{L}(t')\delta\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle_{q0}^{t}$$

$$-\sum_{cd}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{gn}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')\frac{\partial}{\partial\boldsymbol{r}''}\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')\big]_{cd}\langle\delta\hat{n}_{d}(\boldsymbol{r}''')\rangle^{t'}dt'$$

$$+\sum_{cd}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{gR}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')\frac{\partial}{\partial\boldsymbol{r}''}\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')\big]_{cd}\langle\delta\bar{\boldsymbol{M}}_{d}(\boldsymbol{r}'')\rangle^{t'}dt'$$

$$+\sum_{cd}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{gM}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')\big(\big[\tilde{\Phi}_{\bar{M}\bar{M}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')\big]_{cd}\langle\delta\bar{\boldsymbol{M}}_{d}(\boldsymbol{r}''')\rangle^{t'}+\beta\boldsymbol{B}(\boldsymbol{r}',t')\big)dt'$$

$$+\sum_{dcc'd'}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int d\boldsymbol{r}'''''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{gG}^{abcd}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{G}\bar{G}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''',\boldsymbol{r}''''')\big]_{cdc'd'}\langle\delta\overset{\overleftrightarrow{}}{\bar{G}}_{c'd'}(\boldsymbol{r}'''',\boldsymbol{r}''''')\rangle^{t'}dt'$$

$$+\sum_{dcc'd'}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int d\boldsymbol{r}'''''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{gg}^{abcd}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}''\boldsymbol{r}''';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''',\boldsymbol{r}''''')\big]_{cdc'd'}\langle\delta\bar{g}_{c'd'}(\boldsymbol{r}'''',\boldsymbol{r}''''')\rangle^{t'}dt', \tag{37}$$

where $\langle\ldots\rangle_{q0}^{t}=\mathrm{Sp}(\ldots\rho_{q}^{0}(t))$, $\bar{D}_{lj}$ are the transfer kernels and functions of reactions $\bar{K}_{ljk}$, $\bar{K}_{ljks}$, in which the averaging operation is performed with an equilibrium statistical operator (19), $\frac{\partial}{\partial\boldsymbol{r}}\equiv\mathrm{grad}_{\boldsymbol{r}}$. The obtained system of transfer equations is closed and contains the non-dissipative and dissipative contributions, which describe non-Markov diffusion, magneto-diffusion and reaction catalytic processes. If magnetic processes are not formally taken into account, we obtain a system of equations for description of reaction-diffusion processes that were obtained in one form or another [42–44]:

$$\frac{\partial}{\partial t}\langle\delta\hat{n}_{a}(\boldsymbol{r})\rangle^{t}=-\sum_{b}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\frac{\partial}{\partial\boldsymbol{r}}\bar{D}_{nn}^{ab}(\boldsymbol{r},\boldsymbol{r}';t,t')\frac{\partial}{\partial\boldsymbol{r}'}[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}',\boldsymbol{r}'')]_{bc}\langle\delta\hat{n}_{c}(\boldsymbol{r}'')\rangle^{t'}dt'$$

$$-\sum_{bc}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\frac{\partial}{\partial\boldsymbol{r}}\bar{K}_{ng}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''')\big]_{bcdc'}\langle\delta\bar{g}_{dc'}(\boldsymbol{r}''',\boldsymbol{r}'''')\rangle^{t'}dt', \tag{38}$$

$$\frac{\partial}{\partial t}\langle\delta\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle^{t}=\langle i\hat{L}(t')\delta\bar{g}_{ab}(\boldsymbol{r},\boldsymbol{r}')\rangle_{q0}^{t}$$

$$-\sum_{cd}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{gn}^{abc}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';t,t')\frac{\partial}{\partial\boldsymbol{r}''}\big[\tilde{\Phi}_{nn}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''')\big]_{cd}\langle\delta\hat{n}_{d}(\boldsymbol{r}''')\rangle^{t'}dt'$$

$$+\sum_{dcc'd'}\int d\boldsymbol{r}''\int d\boldsymbol{r}'''\int d\boldsymbol{r}''''\int d\boldsymbol{r}'''''\int_{-\infty}^{t}e^{\varepsilon(t'-t)}\bar{K}_{gg}^{abcd}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}''\boldsymbol{r}''';t,t')$$

$$\times\big[\tilde{\Phi}_{\bar{g}\bar{g}}^{-1}(\boldsymbol{r}'',\boldsymbol{r}''',\boldsymbol{r}'''',\boldsymbol{r}''''')\big]_{cdc'd'}\langle\delta\bar{g}_{c'd'}(\boldsymbol{r}'''',\boldsymbol{r}''''')\rangle^{t'}dt'. \tag{39}$$

4. Conclusions

In this paper a statistical description of catalytic oxidation processes is proposed taking into account the reaction–diffusion processes for magnetoactive ions (anions), atoms adsorbed on the metal surface taking into account electronic subsystem. The quantum-classical model for description of reaction–diffusion processes for magnetoactive ions and atoms adsorbed on the metal surface is considered for the purpose of its further application to studies of hydrogen oxidation processes on the surface of magnetoactive metals. As a result, the Hamiltonian of the system is constructed, which takes into account the magneto-dipole nature of ions, electrons, atoms interaction and chemical catalytic bond between the reagents adsorbed on the surface of magnetoactive metal. To describe statistically and obtain reaction-diffusion equations, the main parameters of the abbreviated description are determined in the method of nonequilibrium statistical Zubarev operator [35, 36]. The basic non-Markov transfer equations are obtained for the abbreviated description parameters of reaction-diffusion processes for magnetoactive ions and atoms adsorbed on the metal surface. Weakly nonequilibrium reaction–diffusion processes are also considered. In this case, the obtained system of transfer equations is closed and contains the non-dissipative and dissipative contributions, which describe non-Markov diffusion, magneto-diffusion and reaction catalytic processes. In the next article we will apply specifically the obtained transfer equations to description of hydrogen oxidation processes.

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Статистичний підхід до теоретичного опису процесів каталітичної оксидації водню. Основні рівняння

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Запропоновано статистичний опис процесів каталітичної оксидації водню з врахуванням реакційно-дифузійних процесів для магнітоактивних іонів, атомів адсорбованих на поверхні металу. Отримано основні немарковські рівняння переносу для параметри скороченого опису реакційно-дифузійнійних процесів для магнітоактивних іонів, атомів адсорбованих на поверхні металу у методі нерівноважного статистичного оператора Зубарєва. Розглянуто також слабонерівноважні реакційно-дифузійні процеси.

Ключові слова: *реакційно-дифузійні процеси, немарковські рівняння, метод нерівноважного статистичного оператора.*