

## NONEQUILIBRIUM STATISTICAL OPERATOR METHOD AND GENERALIZED KINETIC EQUATIONS

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*We consider some principal problems of nonequilibrium statistical thermodynamics in the framework of the Zubarev nonequilibrium statistical operator approach. We present a brief comparative analysis of some approaches to describing irreversible processes based on the concept of nonequilibrium Gibbs ensembles and their applicability to describing nonequilibrium processes. We discuss the derivation of generalized kinetic equations for a system in a heat bath. We obtain and analyze a damped Schrödinger-type equation for a dynamical system in a heat bath. We study the dynamical behavior of a particle in a medium taking the dissipation effects into account. We consider the scattering problem for neutrons in a nonequilibrium medium and derive a generalized Van Hove formula. We show that the nonequilibrium statistical operator method is an effective, convenient tool for describing irreversible processes in condensed matter.*

**Keywords:** nonequilibrium statistical physics, irreversible process, nonequilibrium statistical operator method, open system, generalized kinetic equation, damped Schrödinger-type equation, neutron scattering, generalized Van Hove formula

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*This paper is dedicated to the memory of D. N. Zubarev, who was the supervisor of my candidate's dissertation and in much determined my future circle of interests.*

### 1. Introduction

The purpose of statistical mechanics is to create a consistent, effective formalism for describing the macroscopic behavior of multiparticle systems based on the microscopic theory. A rather effective, reliable approach that allows describing a large variety of phenomena in systems such as fluids, gases, and solids was formulated in statistical mechanics. Statistical mechanics also verifies such thermodynamic concepts as heat, temperature, and entropy based on the laws of the microscopic behavior of particles.

The purpose of any theory is to describe reality. It is clear that real systems are open systems that can be regarded as closed only approximately. The central problem of nonequilibrium statistical mechanics is to derive evolution equations for a given system consistently starting from reversible equations of motion. Nonequilibrium statistical thermodynamics provides approaches and tools for describing the irreversible processes in real systems in the framework of a unified theoretical method that allows calculating the transport coefficients characterizing the evolution of nonequilibrium processes (albeit approximately).

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We note that one of the fundamental thermodynamic laws (the second law of thermodynamics) differs quite significantly from other general physical laws. The second law is formulated as an inequality, not an equality. This inequality becomes an equality in the limit of reversible processes. But we know that there are obstacles to the practical realization of this limit. By definition, a reversible process is a process such that the thermodynamic system never deviates significantly from the equilibrium. Because any process takes a finite time, there are unavoidable perturbations affecting the equilibrium. Therefore, deriving reliable, exact evolution equations is quite difficult. We mention a specific aspect of the concept of time in this context. We sometimes say that the time in thermodynamics is manifested not as a quantity itself but only as an indicator of the sense of a quantity: the change in entropy.

For calculating transport coefficients, there are many different methods, which are typically restricted by certain applicability conditions. For instance, the most widely used approach, based on the Boltzmann equation, is applicable to a highly rarefied gas of pointlike particles.

Different schemes for describing kinetic phenomena and transport processes have been proposed in recent decades [1]–[13]. This research direction is actively developing and has many different aspects [14]–[18]. A large contribution to developing modern methods of equilibrium and nonequilibrium statistical mechanics was made by Academician Bogoliubov in [1]–[3]. In what follows, we briefly discuss some of these approaches, mainly those that use the method of the nonequilibrium Gibbs ensemble. We concentrate on the nonequilibrium statistical operator (NSO) method developed by Zubarev [5], [14], [15] and on obtaining generalized kinetic equations in the framework of this approach.

## 2. Equilibrium and nonequilibrium ensemble methods

The task of statistical mechanics is to describe observable equilibrium and nonequilibrium properties of multiparticle systems theoretically based on their molecular content, their specific intermolecular interaction, and the nature of their external environment [19], [20]. The universal tool of equilibrium statistical mechanics was developed by Gibbs [21] and is called the Gibbs ensemble method. The Gibbs method has a high degree of generality and a quite large applicability domain in problems of equilibrium statistical mechanics. The concepts and approaches of this method have diverse applications in various fields [15], [16].

The ensemble is characterized by a distribution function  $f(\mathbf{p}, \mathbf{q})$ , which in the case of classical mechanics must satisfy the Liouville equation

$$\frac{df}{dt} = 0. \quad (2.1)$$

This dynamical requirement reflects the fact that the points in the phase space  $(\mathbf{p}, \mathbf{q})$  representing the system state in an ensemble do not interact with each other; moreover, the phase space volume is preserved. The ensemble method also assumes equiprobabilities of microstates in isolated systems [15], [22], [23].

We note that the concepts of the Gibbs distribution [24] and the Gibbs state play an important role in considering the equilibrium properties of statistical ensembles. The Gibbs distribution in probability theory and mathematical statistical mechanics [15], [16], [22], [23] is defined as the probability distribution describing the configuration statistics of a multiparticle system in thermodynamic equilibrium. It remains invariant during the further evolution of the system. Therefore, for a system in statistical equilibrium, there is a Gibbs distribution function, which can be used to calculate the mean of any dynamical quantity over the ensemble. In contrast, a similar universal distribution has not been formulated for irreversible processes. Numerous approximate models and methods have been applied [5], [15], [16], and mechanical and thermal perturbations causing nonequilibrium processes in a system have been considered [20], [15], [18]. Mechanical perturbations can be expressed as certain contributions to the system Hamiltonian; in this case, the deviations from equilibrium due to such contributions can be described based on perturbation theory.

The linear response method developed by Kubo [5], [15], [16], [20] allows calculating the transport coefficients under mechanical perturbations, such as an external electric field. This allows finding a compact expression for the conductivity in terms of correlation functions. At the same time, being gradients of density and temperature, such thermal perturbations cannot be consistently expressed in terms of perturbative contributions to the Hamiltonian.

In the standard thermodynamic approach, a small number of parameters macroscopically defining the ensemble are used to describe the properties of a uniform equilibrium system [5]. To describe irreversible processes in systems that deviate very slightly from the thermal equilibria, the following technique can be used. We assume that we can divide the system into a set of certain small subsystems, each of which is in local equilibrium [5], [15], [16]. In other words, each of these subsystems can be regarded as a separate thermodynamic system characterized by a small number of physical variables describing its state.

Two mutually related problems are usually considered in the statistical mechanics of transport processes: revealing the mechanism for approaching equilibrium and representing the microscopic properties in terms of macroscopic fluxes. One of the effective approaches to these problems is the Zwanzig approach [8], [9], [10], [25]. It is based on the reformulated Gibbs method and uses projection operators in the space of all possible ensemble densities (or distribution functions) to split the ensemble density into the relevant part (which allows calculating the means of certain quantities over an ensemble) and the remaining irrelevant part. Such a split is a generalization of a known split of the density matrix into the diagonal and nondiagonal parts, which is standardly used to derive the kinetic master equation. It was shown that the relevant part satisfies a kinetic equation that is a generalization of previously obtained master equations, in particular, the Van Hove equation.

The approach related to constructing nonequilibrium ensembles was developed by Bergmann and Lebowitz [26]–[29]. There are many methods for constructing such ensembles, and the distribution function  $\rho(\mathbf{r}_1, \dots, \mathbf{r}_n, \mathbf{p}_1, \dots, \mathbf{p}_n, t)$  characterizing the ensemble state is therefore not defined uniquely. This function must be chosen such that the mean over the ensemble corresponds exactly to the incomplete information about the system state at a given time. The subsequent system evolution is modeled as the behavior averaged over all elements of a representative ensemble.

The accurate definition of a nonequilibrium system state is a rather complicated problem because this state cannot be characterized uniquely. Nevertheless, a detailed consideration in certain cases leads to establishing various time scales during the system evolution [1]–[3], [5]. Moreover, the local equilibrium (quasiequilibrium) distribution and nonequilibrium distribution can often be regarded as having similar structures and functional dependences on the system parameters. This leads to the possibility of a so-called reduced description, in whose framework a rather wide class of transport processes can be described approximately using a certain finite number of macroscopic quantities or relevant variables [5]. In this case, we should remember that for the system to reach a stable state or stay in a nonequilibrium steady state, it must be not isolated but must be in contact with an environment (a system of heat baths), which provides the presence of thermal and other gradients in the system. This was emphasized in papers by Bergmann and Lebowitz [26]–[29], where nonequilibrium solutions for some simple systems in the framework of the nonequilibrium ensemble approach were found and a simple method (of the relaxation type) for constructing the approximate stationary solutions was proposed. But this program turned out to be not entirely successful. The basic inconvenience of this approach is the need for detailed manipulation of the interaction between the system and the heat bath.

Another method, which is closer to the NSO method, was developed by McLennan [6]. It is based on introducing external (nonconservative) forces describing the effect of the environment or heat bath on a given system. In other words, we consider the finite real perturbations due to a heat bath that lead to the irreversible system behavior. Numerous papers on this subject emphasize the need to develop a consistent

theory describing the smoothing of the distribution function in the phase space, which accounts for the increase of entropy in open nonequilibrium systems. This means that the corresponding averaging of the distribution function (statistical operator) plays an important role. These questions have great significance in studying the ergodicity of dynamical and statistical systems [5], [15], [16]. In this context, we note that effective averaging methods in describing complex (nonlinear) systems were developed by Bogoliubov and other authors [30]–[33]. It was noted in [34] that the mixing property arising in ergodicity theory is not a necessary condition for statistical systems with any finite values of the volume and particle number. Only the behavior of the limit averages of macroscopic quantities as  $t \rightarrow \infty$  after the thermodynamic limit transition is important [5], [15], [16]. In [30], [31], an effective averaging method that allows obtaining asymptotic solutions of a differential equation without secular terms was developed in the framework of the perturbation theory in the small parameter  $\varepsilon$ . In this approach, the basic goal is to find a transformation of the variables that allows splitting them into slow and fast variables.

A very effective example of this approach is the paper by Bogoliubov and Zubarev [35]. The averaging method proposed in [30], [31] has a wide application in various problems of dynamical systems theory [30]–[33] and also in problems of statistical mechanics and condensed matter theory [5], [15], [16]. These ideas also stimulated the development of the NSO method [5], which naturally includes ideas about both the presence of various time and energy scales in multiparticle systems and the corresponding reduced description in terms of a small set of relevant variables [5]. In this context, the time-averaging procedure describing the smoothing of the distribution function [5] and the set of relevant variables plays an important role.

### 3. The NSO method

The general idea of the NSO method [5], [14] is that a certain set of parameters  $\{F_m(t)\}$  suffices for describing a nonequilibrium system state at not very small time scales and, in addition, a particular solution  $\rho(t, 0)$  of Liouville equation (2.1) depending on time only via the quantities  $F_m(t)$  can be found. The first argument of  $\rho(t, 0)$  indicates the implicit time dependence. We assume that a nonequilibrium statistical ensemble can be characterized by a small set of relevant operators  $P_m(t)$  (quasi-integrals of motion) and that the NSO is a functional of these operators,

$$\rho(t) = \rho\{\dots, P_m(t), \dots\}. \quad (3.1)$$

It can be shown [5] that if the statistical operator  $\rho(t, 0)$  satisfies the Liouville equation, then it coincides with

$$\rho(t) = \exp\left(\Lambda(t) - \int_{-\infty}^0 dt_1 \sum_m G_m(t, t_1) P_m(t_1)\right), \quad \Lambda(t) = 1 - \lambda(t), \quad (3.2)$$

where

$$\begin{aligned} G_m(t, t_1) &= \varepsilon e^{\varepsilon t_1} F_m(t + t_1), \\ \Lambda(t) &= \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \lambda(t + t_1) = \lambda(t) - \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \dot{\lambda}(t + t_1). \end{aligned} \quad (3.3)$$

We rewrite (3.2) in the form

$$\begin{aligned} \rho &= \exp(\overline{\log \rho_q(t)}) = \exp\left(\varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \exp\left(\frac{iHt_1}{\hbar}\right) \log \rho_q(t + t_1) \exp\left(\frac{-iHt_1}{\hbar}\right)\right) = \\ &= \exp(\overline{-S(t, 0)}) = \exp\left(-\varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} S(t + t_1, t_1)\right) = \\ &= \exp\left(-S(t, 0) + \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \dot{S}(t + t_1, t_1)\right), \end{aligned} \quad (3.4)$$

where the bar denotes the invariant part of an operator [5],

$$\begin{aligned}\rho_q(t) &= \exp\left(\Omega(t) - \sum_m F_m(t)P_m\right) \equiv \exp(-S(t, 0)), \\ \Omega(t) &= \log \text{Tr} \exp\left(-\sum_m F_m(t)P_m\right),\end{aligned}\tag{3.5}$$

and  $S(t, t_1)$  satisfies the equations

$$\begin{aligned}\dot{S}(t, 0) &= \frac{\partial S(t, 0)}{\partial t} + \frac{1}{i\hbar}[S(t, 0), H], \\ \dot{S}(t, t_1) &= \exp\left(\frac{iHt_1}{\hbar}\right)\dot{S}(t, 0)\exp\left(\frac{-iHt_1}{\hbar}\right).\end{aligned}\tag{3.6}$$

Here,  $\rho_q$  is the *quasiequilibrium statistical operator*, corresponding to the extreme value of the information entropy  $S = -\text{Tr}(\rho \log \rho)$  [5], [15], [36]–[39] under the additional conditions of constant  $\text{Tr}(\rho P_m) = \langle P_m \rangle_q$  with  $\text{Tr} \rho = 1$ . In this case,

$$\frac{\delta \Phi}{\delta F_m} = -\langle P_m \rangle_q, \quad \langle \cdot \rangle_q = \text{Tr}(\rho_q \cdot),\tag{3.7}$$

where

$$\Phi(\rho) = -\text{Tr}(\rho \log \rho) - \sum_m F_m \text{Tr}(\rho P_m) + \lambda \text{Tr} \rho, \quad \langle P_m \rangle^t = \langle P_m \rangle_q^t.\tag{3.8}$$

We again emphasize that the NSO method, as noted above, is essentially based on an analogy with nonlinear mechanics [30]–[33]. A nonlinear system tending to a limit cycle “forgets” its initial conditions. Therefore, the variables necessary for characterizing the system (relevant operators) depending on time via  $F_m(t)$  must be constructed by taking the part of the operators (which are included in the logarithm of the statistical operator) that is invariant under motion with the Hamiltonian  $H$ . We explain this in more detail.

By definition, taking the invariant part of the operator  $F_m(t)P_m$  yields

$$\begin{aligned}B_m(t) &= \overline{F_m(t)P_m} = \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} F_m(t+t_1)P_m(t_1) = \\ &= F_m(t)P_m - \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} (F_m(t+t_1)\dot{P}_m(t_1) + \dot{F}_m(t+t_1)P_m(t_1)).\end{aligned}\tag{3.9}$$

Here,  $\varepsilon \rightarrow 0$  and

$$\dot{P}_m = \frac{1}{i\hbar}[P_m, H], \quad \dot{F}_m(t) = \frac{dF_m(t)}{dt}.\tag{3.10}$$

We emphasize that the parameter  $\varepsilon > 0$  tends to zero only after the thermodynamic limit transition [22], [23]. The operators  $B_m(t)$  satisfy the Liouville equation in the limit  $\varepsilon \rightarrow 0$ :

$$\frac{\partial B_m}{\partial t} - \frac{1}{i\hbar}[B_m, H] = \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} (F_m(t+t_1)\dot{P}_m(t_1) + \dot{F}_m(t+t_1)P_m(t_1)).\tag{3.11}$$

Therefore, the operation of taking the invariant part leads to smoothing the oscillating terms.

We note that a similar procedure is used in formal scattering theory [5] and allows imposing boundary conditions that eliminate advanced solutions of the Schrödinger equation [5], [15]. This is especially clear

when the parameters  $F_m(t)$  are independent of time. Differentiating the operator  $\overline{P_m}$  with respect to time yields

$$\frac{\partial \overline{P_m(t)}}{\partial t} = \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \dot{P}_m(t+t_1). \quad (3.12)$$

The quantities  $\overline{P_m(t)}$  can be regarded as integrals (or quasi-integrals) of motion although they are conserved only in the limit  $\varepsilon \rightarrow 0$ . In our context, this procedure leads to selecting only the retarded solutions of the Liouville equation.

The quantum (and also classical) Liouville equation is invariant under a time reversal. It is well known that the Bogoliubov concept of quasiaverages [40]–[42] has great significance in equilibrium statistical mechanics. According to this concept, infinitesimal perturbations can have a large effect on a system if they break any symmetry and thus remove degeneration (or quasidegeneration). As a result, their effect can be finite if they tend to zero after the thermodynamic limit transition. Zubarev [41] showed that the concept of symmetry-breaking perturbations and quasiaverages is also meaningful in the theory of irreversible processes [5]. The method for constructing the NSO [5] gains great transparency and depth in the framework of the concept of quasiaverages. The general idea in [41] is to consider infinitesimal sources breaking the symmetry of the Liouville equation.

It can be shown [41] that  $\rho(t, 0)$  satisfies the Liouville equation but with an infinitesimal source in the right-hand side. This source is proportional to  $\varepsilon$ , which tends to zero after the thermodynamic limit transition. Indeed, we consider the equation

$$\frac{\partial \rho_\varepsilon}{\partial t} + \frac{1}{i\hbar} [\rho_\varepsilon, H] = -\varepsilon(\rho_\varepsilon - \rho_q) \quad (3.13)$$

or, written differently,

$$\frac{\partial \log \rho_\varepsilon}{\partial t} + \frac{1}{i\hbar} [\log \rho_\varepsilon, H] = -\varepsilon(\log \rho_\varepsilon - \log \rho_q), \quad (3.14)$$

where  $\varepsilon \rightarrow 0$  after the thermodynamic limit transition. Equation (3.13) is an analogue of the corresponding equation in quantum scattering theory [5]. Introducing infinitesimal sources in the Liouville equation corresponds to imposing the boundary conditions

$$\exp\left(\frac{iHt_1}{\hbar}\right) (\rho(t+t_1) - \rho_q(t+t_1)) \exp\left(-\frac{iHt_1}{\hbar}\right) \rightarrow 0. \quad (3.15)$$

Here,  $t_1 \rightarrow -\infty$  after the thermodynamic limit transition.

It was shown in [43]–[45] that the operator  $\rho_\varepsilon$  has the form

$$\rho_\varepsilon(t, t) = \varepsilon \int_{-\infty}^t dt_1 e^{\varepsilon(t_1-t)} \rho_q(t_1, t_1) = \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \rho_q(t+t_1, t+t_1). \quad (3.16)$$

Here, the first argument in the function denotes the implicit time dependence via the parameters  $F_m(t)$ , and the second denotes the time dependence via the Heisenberg representation. The sought statistical operator can be defined as

$$\rho_\varepsilon = \rho_\varepsilon(t, 0) = \overline{\rho_q(t, 0)} = \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \rho_q(t+t_1, t_1). \quad (3.17)$$

As a result, the NSO becomes

$$\begin{aligned} \rho &= Q^{-1} \exp\left(-\sum_m B_m\right) = Q^{-1} \exp\left(-\sum_m \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} F_m(t+t_1) P_m(t_1)\right) = \\ &= Q^{-1} \exp\left(-\sum_m F_m(t) P_m + \sum_m \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} (\dot{F}_m(t+t_1) P_m(t_1) + F_m(t+t_1) \dot{P}_m(t_1))\right). \end{aligned} \quad (3.18)$$

We can write Eq. (3.14) in the form

$$\frac{d}{dt}(e^{\varepsilon t} \log \rho(t, t)) = \varepsilon e^{\varepsilon t} \log \rho_q(t, t), \quad (3.19)$$

where

$$\log \rho(t, t) = U^\dagger(t, 0) \log \rho(t, 0) U(t, 0), \quad U(t, 0) = \exp\left(\frac{iHt}{\hbar}\right). \quad (3.20)$$

Integrating (3.19) over the interval  $(-\infty, 0)$ , we obtain

$$\log \rho(t, t) = \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \log \rho_q(t + t_1, t + t_1). \quad (3.21)$$

We assume that  $\lim_{\varepsilon \rightarrow +0} \log \rho(t, t) = 0$ . As a result, we have

$$\rho(t, 0) = \exp\left(-\varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \log \rho_q(t + t_1, t_1)\right) = \exp(\overline{\log \rho_q(t, 0)}) \equiv \exp(\overline{-S(t, 0)}).$$

The mean of any dynamical variable  $A$  can be calculated as

$$\langle A \rangle = \lim_{\varepsilon \rightarrow +0} \text{Tr}(\rho(t, 0)A), \quad (3.22)$$

and we see that it is just the quasiaverage. The normalization of the quasiequilibrium distribution  $\rho_q$  is preserved under the conditions

$$\text{Tr}(\rho(t, 0)P_m) = \langle P_m \rangle = \langle P_m \rangle_q, \quad \text{Tr} \rho = 1. \quad (3.23)$$

We can therefore state that the effect of irreversibility is closely related to breaking the time symmetry [15] and, in a certain sense, to the idea of quasiaverages in statistical mechanics [40]–[42].

Before discussing kinetic equations, we briefly discuss the hierarchy of time scales in nonequilibrium processes. A significant advantage of the NSO method is that the existence of different time scales is emphasized in it from the very beginning. We assume that the Hamiltonian of our system can be represented in the form  $H = H_0 + V$ , where  $H_0$  is an unperturbed Hamiltonian and  $V$  describes a weak perturbation. This split of the original Hamiltonian is not quite unique and depends on the system feature considered. It is important that the choice of the operator  $H_0$  defines a short-time scale  $\tau_0$ . This choice is determined by the fact that the nonequilibrium system state for  $t \gg \tau_0$  can be described (with reasonable accuracy) using some finite set of operators  $P_m$ .

We assume that after the short time  $\tau_0$  (fast stage), the system can reach an incomplete equilibrium or a quasiequilibrium. In this case, the basic assumption is that the system state is completely determined using the quasi-integrals of motion, which are the inner system parameters. Typical relaxation times of these parameters are much longer than  $\tau_0$ . With a high degree of likelihood, we can then state that even if the quasi-integrals do not have certain equilibrium values at the initial instant, then these fast-varying variables become functions of external parameters and of quasi-integrals of motion after the time  $\tau_0$ . It is important that this functional relation is independent of the initial values of these variables. In other words, the operators  $P_m$  must be chosen such that they satisfy the condition

$$[P_k, H_0] = \sum_l c_{kl} P_l, \quad (3.24)$$

where  $c_{kl}$  are some coefficients (complex numbers). We should write the evolution equation for only this set of relevant operators. We note that the relevant operators can be either scalars or vectors.

The equations of motion for means of the other (nonrelevant) operators (other physical variables) follow in some sense from the evolution equations for the relevant operators. Moreover, relation (3.24) leads to an infinite chain of operator equalities. For times  $t \leq \tau_0$ , the nonequilibrium means of these operators are fast oscillating, and they become functions of the means for times  $t > \tau_0$ .

## 4. Generalized kinetic equations

The NSO method [5] has wide application in various problems of statistical mechanics. Pokrovskii [46] contributed greatly to the development of kinetic equation theory in the framework of the NSO method. Generalized kinetic transport equations describing the evolution of  $\langle P_m \rangle$  and  $F_m(t)$  can be obtained by averaging the equations of motion for  $P_m$  with the found NSO:

$$\langle P_m \rangle = -\frac{\delta\Omega}{\delta F_m(t)}, \quad F_m(t) = \frac{\delta S}{\delta \langle P_m \rangle}. \quad (4.1)$$

The generalized transport equations are

$$\langle \dot{P}_m \rangle = -\sum_n \frac{\delta^2\Omega}{\delta F_m(t) \delta F_n(t)} \dot{F}_n(t), \quad \dot{F}_m(t) = \sum_n \frac{\delta^2 S}{\delta \langle P_m \rangle \delta \langle P_n \rangle} \langle \dot{P}_n \rangle. \quad (4.2)$$

In addition, the entropy production can be written as

$$\dot{S}(t) = \langle \dot{S}(t, 0) \rangle = -\sum_m \langle \dot{P}_m \rangle F_m(t) = -\sum_{n,m} \frac{\delta^2\Omega}{\delta F_m(t) \delta F_n(t)} \dot{F}_n(t) F_m(t). \quad (4.3)$$

Equations (4.2) are mutually conjugate and together with (4.3) form a complete system of equations for  $\langle P_m \rangle$  and  $F_m$ .

Following [46], we write the kinetic equations for a system with a weak interaction. The Hamiltonian is  $H = H_0 + V$ , where  $H_0$  is the Hamiltonian of noninteracting particles (or quasiparticles) and  $V$  is the interaction operator. As relevant operators, we chose the set of  $P_k$  in the form  $a_k^\dagger a_k$  or  $a_k^\dagger a_{k+q}$ . Here,  $a_k^\dagger$  and  $a_k$  are the creation and annihilation operators (either Fermi or Bose). The starting equations are the equations of motion

$$\dot{P}_k = \frac{1}{i\hbar} [P_k, H]. \quad (4.4)$$

Below, we assume that relation (3.24) holds.

In accordance with (3.18), we have

$$\rho = Q^{-1} \exp\left(-\sum_k F_k(t) P_k + \sum_k \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} (\dot{F}_k(t+t_1) P_k(t_1) + F_k(t+t_1) \dot{P}_k(t_1))\right).$$

We also take  $\langle P_k \rangle = \langle P_k \rangle_{\mathfrak{q}}$  into account. Generalized kinetic equations [46] for  $\langle P_k \rangle$  can be written as

$$\frac{d\langle P_k \rangle}{dt} = \frac{1}{i\hbar} \langle [P_k, H] \rangle = \frac{1}{i\hbar} \sum_l c_{kl} \langle P_l \rangle + \frac{1}{i\hbar} \langle [P_k, V] \rangle. \quad (4.5)$$

The right-hand sides of these equations contain a generalized collision integral, which can be written using an expansion in powers of  $V$  as

$$\frac{d\langle P_k \rangle}{dt} = L_k^0 + L_k^1 + L_k^{21} + L_k^{22}, \quad (4.6)$$

where

$$\begin{aligned} L_k^0 &= \frac{1}{i\hbar} \sum_l c_{kl} \langle P_l \rangle_{\mathfrak{q}}, & L_k^1 &= \frac{1}{i\hbar} \langle [P_k, V] \rangle_{\mathfrak{q}}, \\ L_k^{21} &= \frac{1}{\hbar^2} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle [V(t_1), [P_k, V]] \rangle_{\mathfrak{q}}, \\ L_k^{22} &= \frac{1}{\hbar^2} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \left\langle \left[ V(t_1), i\hbar \sum_l P_l \frac{\partial L_k^1(\dots, \langle P_l \rangle, \dots)}{\partial \langle P_l \rangle} \right] \right\rangle_{\mathfrak{q}}. \end{aligned} \quad (4.7)$$

We can similarly find terms corresponding to the higher orders  $V^3$ ,  $V^4$ , etc.



**4.1. Generalized kinetic equations for a system in a heat bath.** Equations (4.5) were generalized in [47] to a system interacting with a heat bath. The concept of a heat bath is rather complicated and has specific features [48]. Normally, a heat bath is defined as a system with an effectively infinite number of degrees of freedom. A heat bath maintains a desired temperature of the considered system. Following Bogoliubov [3], we regard a heat bath as a randomizing source for a small subsystem (which can be a single particle in the limit case). An example of such systems is an atomic or molecular system interacting with an electromagnetic field or a system of nuclear or electron spins interacting with a crystal lattice.

The complete system can be described by the Hamiltonian

$$H = H_1 + H_2 + V, \quad (4.8)$$

where

$$H_1 = \sum_{\alpha} E_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}, \quad V = \sum_{\alpha, \beta} \Phi_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta}, \quad \Phi_{\alpha\beta} = \Phi_{\beta\alpha}^{\dagger}. \quad (4.9)$$

Here,  $H_1$  is the Hamiltonian of the small subsystem,  $a_{\alpha}^{\dagger}$  and  $a_{\alpha}$  are the creation and annihilation operators of quasiparticles with the energies  $E_{\alpha}$  in the small subsystem,  $V$  is the interaction operator between the small subsystem and the heat bath, and  $H_2$  is the heat bath Hamiltonian, which we do not write explicitly. The operators  $\Phi_{\alpha\beta}$  act on the heat bath variables. We assume that the system state can be characterized by the set of operators  $\langle P_{\alpha\beta} \rangle = \langle a_{\alpha}^{\dagger} a_{\beta} \rangle$  and the heat bath state can be described by the operator  $\langle H_2 \rangle$ . Here,  $\langle \bullet \rangle$  denotes averaging with the NSO, which is defined below.

We write the quasiequilibrium operator in the form

$$\rho_{\text{q}}(t) = \exp(-S(t, 0)), \quad (4.10)$$

where

$$S(t, 0) = \Omega(t) + \sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t) + \beta H_2, \quad \Omega(t) = \log \text{Tr} \exp\left(-\sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t) - \beta H_2\right).$$

Here,  $F_{\alpha\beta}(t)$  are the thermodynamic parameters conjugate to  $P_{\alpha\beta}$ , and  $\beta$  is the inverse temperature of the heat bath. All operators are considered in the Heisenberg representation. We write the NSO as

$$\rho(t) = \exp(-\overline{S(t, 0)}), \quad (4.11)$$

where

$$\overline{S(t, 0)} = \varepsilon \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \left( \Omega(t + t_1) + \sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t) + \beta H_2 \right). \quad (4.12)$$

The parameters  $F_{\alpha\beta}(t)$  are defined by the condition  $\langle P_{\alpha\beta} \rangle = \langle P_{\alpha\beta} \rangle_{\text{q}}$ . Deriving the kinetic equations, we use the expansion in the parameter of the small perturbation  $V$  and also assume that the equality  $\langle \Phi_{\alpha\beta} \rangle_{\text{q}} = 0$  holds.

For convenience in the further analysis, we rewrite  $\rho_{\text{q}}$  as

$$\rho_{\text{q}} = \rho_1 \otimes \rho_2 = Q_{\text{q}}^{-1} \exp(-L_0(t)), \quad (4.13)$$

where

$$\begin{aligned} \rho_1 &= Q_1^{-1} \exp\left(-\sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t)\right), & Q_1 &= \text{Tr} \exp\left(-\sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t)\right), \\ \rho_2 &= Q_2^{-1} e^{-\beta H_2}, & Q_2 &= \text{Tr} \exp(-\beta H_2), \\ Q_{\text{q}} &= Q_1 Q_2, & L_0 &= \sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t) + \beta H_2. \end{aligned} \quad (4.14)$$

The starting equation is

$$\frac{d\langle P_{\alpha\beta} \rangle}{dt} = \frac{1}{i\hbar} \langle [P_{\alpha\beta}, H] \rangle = \frac{1}{i\hbar} (E_\beta - E_\alpha) \langle P_{\alpha\beta} \rangle + \frac{1}{i\hbar} \langle [P_{\alpha\beta}, V] \rangle, \quad (4.15)$$

where we restrict ourself to terms of the second order in  $V$ . For a system in a heat bath, the kinetic equations written for  $\langle P_{\alpha\beta} \rangle$  are

$$\frac{d\langle P_{\alpha\beta} \rangle}{dt} = \frac{1}{i\hbar} (E_\beta - E_\alpha) \langle P_{\alpha\beta} \rangle - \frac{1}{\hbar^2} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle [[P_{\alpha\beta}, V], V(t_1)] \rangle_{\text{q}}. \quad (4.16)$$

These equations generalize the results in [46] to a system in a heat bath. We can show that the assumption concerning the model form of Hamiltonian (4.8) is insignificant. For arbitrary  $H_1$  and  $V$  and some set of variables  $\langle P_k \rangle$  satisfying the condition  $[H_1, P_k] = \sum_l c_{kl} P_l$ , we can construct the quasiequilibrium statistical operator  $\rho_{\text{q}}$  in the form

$$\rho_{\text{q}} = Q_{\text{q}}^{-1} \exp\left(-\sum_k P_k F_k(t) - \beta H_2\right), \quad (4.17)$$

where  $F_k(t)$  are the parameters conjugate to  $\langle P_k \rangle$ . In this case, the kinetic equations for  $\langle P_k \rangle$  are

$$\frac{d\langle P_k \rangle}{dt} = \frac{i}{\hbar} \sum_l c_{kl} \langle P_l \rangle - \frac{1}{\hbar^2} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle [[P_k, V], V(t_1)] \rangle_{\text{q}}. \quad (4.18)$$

We note that the derived generalized kinetic equations are a useful tool for studying quantum dynamics in condensed matter [15], [16], [18], [49]. One method for studying quantum dynamics is the reduced density matrix method. In this approach, the reduced density matrix can be obtained by taking the average  $\rho^1 = \text{Tr}_2 \rho$  of the complete matrix over the irrelevant heat bath degrees of freedom. A known example of this approach is the Redfield equations for the spin density matrix, which were also obtained (in a generalized form) using the NSO method [15], [16], [49]. Redfield-type equations for  $\langle P_{\alpha\beta} \rangle$  can be written in a general form as

$$\begin{aligned} \frac{d\langle P_{\alpha\beta} \rangle}{dt} &= \frac{1}{i\hbar} (E_\beta - E_\alpha) \langle P_{\alpha\beta} \rangle - \\ &- \sum_{\nu} (K_{\beta\nu} \langle P_{\alpha\nu} \rangle + K_{\alpha\nu}^\dagger \langle P_{\nu\beta} \rangle) + \sum_{\mu,\nu} K_{\alpha\beta,\mu\nu} \langle P_{\mu\nu} \rangle. \end{aligned} \quad (4.19)$$

In structure, they correspond to the Redfield equations for the spin density matrix

$$\frac{\partial \rho^{\alpha\alpha'}}{\partial t} = -i\omega_{\alpha\alpha'} \rho^{\alpha\alpha'} + \sum_{\beta,\beta'} R_{\alpha\alpha'\beta\beta'} \rho^{\beta\beta'} \quad (4.20)$$

in the absence of an external field (the case of a variable external field was considered in [15], [16], [49]). Here,  $\rho^{\alpha\alpha'}$  is the  $\alpha\alpha'$  element of the spin density matrix,  $\omega_{\alpha\alpha'} = (E_\alpha - E_{\alpha'})/\hbar$ ,  $E_\alpha$  is the energy of the spin state  $\alpha$ , and  $R_{\alpha\alpha'\beta\beta'}$  is the so-called ‘‘relaxation matrix’’ (see [15], [16] for the detailed notation).

Returning to Eq. (4.19), we consider the case of the diagonal means  $\langle P_{\alpha\alpha} \rangle$ . As a result, we obtain

$$\frac{d\langle P_{\alpha\alpha} \rangle}{dt} = \sum_{\nu} K_{\alpha\alpha,\nu\nu} \langle P_{\nu\nu} \rangle - (K_{\alpha\alpha} + K_{\alpha\alpha}^\dagger) \langle P_{\alpha\alpha} \rangle, \quad (4.21)$$

where

$$\begin{aligned}
K_{\alpha\alpha,\beta\beta} &= \frac{1}{\hbar^2} J_{\alpha\beta,\beta\alpha} \left( \frac{E_\alpha - E_\beta}{\hbar} \right) = W_{\beta \rightarrow \alpha}, \\
K_{\alpha\alpha} + K_{\alpha\alpha}^\dagger &= \frac{1}{\hbar^2} \sum_\beta J_{\beta\alpha,\alpha\beta} \left( \frac{E_\beta - E_\alpha}{\hbar} \right) = W_{\alpha \rightarrow \beta}.
\end{aligned} \tag{4.22}$$

The quantities  $W_{\beta \rightarrow \alpha}$  and  $W_{\alpha \rightarrow \beta}$  denote the transition probabilities expressed in terms of the spectral intensities  $J$ . Using the properties of the spectral intensities [5], we can verify that the transition probabilities satisfy the detailed balance equations

$$\frac{W_{\beta \rightarrow \alpha}}{W_{\alpha \rightarrow \beta}} = \frac{e^{-\beta E_\alpha}}{e^{-\beta E_\beta}}. \tag{4.23}$$

As a result, we obtain the equation

$$\frac{d\langle P_{\alpha\alpha} \rangle}{dt} = \sum_\nu W_{\nu \rightarrow \alpha} \langle P_{\nu\nu} \rangle - \sum_\nu W_{\alpha \rightarrow \nu} \langle P_{\alpha\alpha} \rangle, \tag{4.24}$$

which has the usual form of the famous Pauli equation (Pauli master equation) for the density matrix [15], [16].

**4.2. Schrödinger-type equation for a dynamical system in a heat bath.** Following [15], [16], [50], we now consider the behavior of a small dynamical subsystem governed by the Hamiltonian  $H_1$  and interacting with a heat bath governed by the Hamiltonian  $H_2$ . As operators characterizing the state of the small subsystem, we choose the operators  $a_\alpha^\dagger$ ,  $a_\alpha$ , and  $n_\alpha = a_\alpha^\dagger a_\alpha$ . In this case, the quasiequilibrium statistical operator  $\rho_q$  becomes

$$\rho_q = \exp \left( \Omega - \sum_\alpha (f_\alpha(t) a_\alpha + f_\alpha^\dagger(t) a_\alpha^\dagger + F_\alpha(t) n_\alpha) - \beta H_2 \right) \equiv \exp(-S(t, 0)), \tag{4.25}$$

where

$$\Omega = \log \text{Tr} \exp \left( - \sum_\alpha (f_\alpha(t) a_\alpha + f_\alpha^\dagger(t) a_\alpha^\dagger + F_\alpha(t) n_\alpha) - \beta H_2 \right). \tag{4.26}$$

Here,  $f_\alpha$ ,  $f_\alpha^\dagger$ , and  $F_\alpha$  play the role of Lagrange multipliers. They are the parameters conjugate to  $\langle a_\alpha \rangle_q$ ,  $\langle a_\alpha^\dagger \rangle_q$ , and  $\langle n_\alpha \rangle_q$ :

$$\langle a_\alpha \rangle_q = - \frac{\delta \Omega}{\delta f_\alpha(t)}, \quad \langle n_\alpha \rangle_q = - \frac{\delta \Omega}{\delta F_\alpha(t)}, \quad \frac{\delta S}{\delta \langle a_\alpha \rangle_q} = f_\alpha(t), \quad \frac{\delta S}{\delta \langle n_\alpha \rangle_q} = F_\alpha(t). \tag{4.27}$$

The quantities  $a_\alpha$  and  $a_\alpha^\dagger$  in the statistical operator can be interpreted as sources of quantum noise [15], [16].

We transform the quasiequilibrium statistical operator into the form  $\rho_q = \rho_1 \otimes \rho_2$ , where

$$\begin{aligned}
\rho_1 &= \exp \left( \Omega_1 - \sum_\alpha (f_\alpha(t) a_\alpha + f_\alpha^\dagger(t) a_\alpha^\dagger + F_\alpha(t) n_\alpha) \right), \\
\Omega_1 &= \log \text{Tr} \exp \left( - \sum_\alpha (f_\alpha(t) a_\alpha + f_\alpha^\dagger(t) a_\alpha^\dagger + F_\alpha(t) n_\alpha) \right), \\
\rho_2 &= \exp(\Omega_2 - \beta H_2), \quad \Omega_2 = \log \text{Tr} \exp(-\beta H_2).
\end{aligned} \tag{4.28}$$

As a result, we obtain expression (4.11) for the NSO  $\rho$ . We assume that the conditions

$$\langle a_\alpha \rangle_q = \langle a_\alpha \rangle, \quad \langle a_\alpha^\dagger \rangle_q = \langle a_\alpha^\dagger \rangle, \quad \langle n_\alpha \rangle_q = \langle n_\alpha \rangle \tag{4.29}$$

are satisfied.

We start from the equations of motion

$$\begin{aligned} i\hbar \frac{d\langle a_\alpha \rangle}{dt} &= \langle [a_\alpha, H_1] \rangle + \langle [a_\alpha, V] \rangle, \\ i\hbar \frac{d\langle n_\alpha \rangle}{dt} &= \langle [n_\alpha, H_1] \rangle + \langle [n_\alpha, V] \rangle. \end{aligned} \quad (4.30)$$

The second order in  $V$  yields

$$\begin{aligned} i\hbar \frac{d\langle a_\alpha \rangle}{dt} &= E_\alpha \langle a_\alpha \rangle + \frac{1}{i\hbar} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle [[a_\alpha, V], V(t_1)] \rangle_{\text{q}}, \\ i\hbar \frac{d\langle n_\alpha \rangle}{dt} &= \frac{1}{i\hbar} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle [[n_\alpha, V], V(t_1)] \rangle_{\text{q}}. \end{aligned} \quad (4.31)$$

Here,  $V(t_1)$  denotes the operator  $V$  in the interaction representation. The expansion yields

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \frac{1}{i\hbar} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \left( \sum_{\beta, \mu, \nu} \langle \Phi_{\alpha\beta} \phi_{\mu\nu}(t_1) \rangle_{\text{q}} \langle a_\beta a_\mu^\dagger a_\nu \rangle_{\text{q}} - \langle \phi_{\mu\nu}(t_1) \Phi_{\alpha\beta} \rangle_{\text{q}} \langle a_\mu^\dagger a_\nu a_\beta \rangle_{\text{q}} \right),$$

where  $\phi_{\mu\nu}(t_1) = \Phi_{\mu\nu}(t_1) \exp((i/\hbar)(E_\mu - E_\nu)t_1)$  or, using another form,

$$\begin{aligned} i\hbar \frac{d\langle a_\alpha \rangle}{dt} &= E_\alpha \langle a_\alpha \rangle + \frac{1}{i\hbar} \sum_{\beta, \mu} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle \Phi_{\alpha\mu} \phi_{\mu\beta}(t_1) \rangle_{\text{q}} \langle a_\beta \rangle + \\ &+ \frac{1}{i\hbar} \sum_{\beta, \mu, \nu} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle [\Phi_{\alpha\nu}, \phi_{\mu\nu}(t_1)] \rangle_{\text{q}} \langle a_\mu^\dagger a_\nu a_\beta \rangle_{\text{q}}. \end{aligned} \quad (4.32)$$

As a result, we obtain

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \frac{1}{i\hbar} \sum_{\beta, \mu} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle \Phi_{\alpha\mu} \phi_{\mu\beta}(t_1) \rangle_{\text{q}} \langle a_\beta \rangle. \quad (4.33)$$

Using the spectral representations for the correlation functions, we can write the equation

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \sum_{\beta} K_{\alpha\beta} \langle a_\beta \rangle, \quad (4.34)$$

where  $K_{\alpha\beta}$  is defined as

$$\frac{1}{i\hbar} \sum_{\mu} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle \Phi_{\beta\mu} \phi_{\mu\nu}(t_1) \rangle_{\text{q}} = \frac{1}{2\pi} \sum_{\mu} \int_{-\infty}^{+\infty} d\omega \frac{J_{\mu\nu, \beta\mu}(\omega)}{\hbar\omega - E_\mu - E_\nu + i\varepsilon} = K_{\beta\nu}. \quad (4.35)$$

Hence, we obtain a Schrödinger-type equation for the mean amplitudes  $\langle a_\alpha \rangle$ . In a certain sense, it is an analogue (or generalization) of the Schrödinger equation for a particle moving in a medium. We consider this analogy in more detail. For this, we write the analogue of the wave function as

$$\psi(\mathbf{r}) = \sum_{\alpha} \chi_{\alpha}(\mathbf{r}) \langle a_{\alpha} \rangle. \quad (4.36)$$

Here,  $\{\chi_\alpha(\mathbf{r})\}$  is the full orthonormalized set of one-particle wave functions for the operator  $(-\hbar^2/2m)\nabla^2 + v(\mathbf{r})$ , and  $v(\mathbf{r})$  is the potential energy. We have the equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\right)\chi_\alpha(\mathbf{r}) = E_\alpha\chi_\alpha(\mathbf{r}). \quad (4.37)$$

The quantity  $\psi(\mathbf{r})$  thus plays the role of the wave function for a particle moving in a medium with friction. In this case, Eq. (4.34) becomes

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\right)\psi(\mathbf{r}) + \int d^3r' K(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}'), \quad (4.38)$$

where the kernel  $K(\mathbf{r}, \mathbf{r}')$  of integral equation (4.38) is

$$K(\mathbf{r}, \mathbf{r}') = \sum_{\alpha, \beta} K_{\alpha\beta}\chi_\alpha(\mathbf{r})\chi_\beta^\dagger(\mathbf{r}') = \frac{1}{i\hbar} \sum_{\alpha, \beta, \mu} \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle \Phi_{\alpha\mu} \phi_{\mu\beta}(t_1) \rangle_{\mathbf{q}} \chi_\alpha(\mathbf{r})\chi_\beta^\dagger(\mathbf{r}').$$

We see that (4.38) can indeed be called the Schrödinger-type equation for a dynamical system in a heat bath. It is interesting that very similar Schrödinger-type equations with nonlocal interaction were used in collision theory [15], [16] to describe particle scattering on an ensemble of many scattering centers. To explicitly show some features of Eq. (4.38), we consider the translation operator  $e^{i\mathbf{q}\mathbf{p}/\hbar}$ , where  $\mathbf{q} = \mathbf{r}' - \mathbf{r}$  and  $\mathbf{p} = -i\hbar\nabla_r$ . We can then write (4.38) as

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\right)\psi(\mathbf{r}) + \sum_p D(\mathbf{r}, \mathbf{p})\psi(\mathbf{r}), \quad (4.39)$$

where

$$D(\mathbf{r}, \mathbf{p}) = \int d^3q K(\mathbf{r}, \mathbf{r} + \mathbf{q})e^{i\mathbf{q}\mathbf{p}/\hbar}. \quad (4.40)$$

It is reasonable to assume that the variation of the wave function  $\psi(\mathbf{r})$  is not very significant over the typical correlation length of the kernel  $K(\mathbf{r}, \mathbf{r}')$ . Using the series expansion for  $e^{i\mathbf{q}\mathbf{p}/\hbar}$ , we then obtain

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) + \text{Re}U(\mathbf{r})\right)\psi(\mathbf{r}) + i\text{Im}U(\mathbf{r})\psi(\mathbf{r}) \quad (4.41)$$

(in the zeroth order), where

$$U(\mathbf{r}) = \text{Re}U(\mathbf{r}) + i\text{Im}U(\mathbf{r}) = \int d^3q K(\mathbf{r}, \mathbf{r} + \mathbf{q}). \quad (4.42)$$

Equation (4.41) has exactly the functional form of the Schrödinger equation with a complex potential known in collision theory [15], [16]. Expanding  $e^{i\mathbf{q}\mathbf{p}/\hbar}$  in a series up to the second order, we then represent Eq. (4.38) in the form [16], [50]

$$\begin{aligned} i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t} = & \left\{ \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\right) + U(\mathbf{r}) - \frac{1}{i\hbar} \int d^3r' K(\mathbf{r}, \mathbf{r} + \mathbf{r}')\mathbf{r}'\mathbf{p} + \right. \\ & \left. + \frac{1}{2} \int d^3r' K(\mathbf{r}, \mathbf{r} + \mathbf{r}') \sum_{i,k=1}^3 r'_i r'_k \nabla_i \nabla_k \right\} \psi(\mathbf{r}). \end{aligned} \quad (4.43)$$

If we introduce the function

$$\mathbf{A}(\mathbf{r}) = \frac{c}{i\hbar e} \int d^3r' K(\mathbf{r}, \mathbf{r} + \mathbf{r}') \mathbf{r}', \quad (4.44)$$

which is an analogue (in a certain sense) of the complex vector potential  $\mathbf{A}$  of an electromagnetic field, and the effective mass tensor [15], [51]

$$\left\{ \frac{1}{M(\mathbf{r})} \right\}_{ik} = \frac{1}{m} \delta_{ik} - \int d^3r' \operatorname{Re} K(\mathbf{r}, \mathbf{r} + \mathbf{r}') r'_i r'_k, \quad (4.45)$$

then we can write (4.43) in the form

$$i\hbar \frac{\partial \psi(\mathbf{r})}{\partial t} = \left\{ -\frac{\hbar^2}{2} \sum_{i,k} \left( \frac{1}{M(\mathbf{r})} \right)_{ik} \nabla_i \nabla_k + v(\mathbf{r}) + U(\mathbf{r}) + \frac{i\hbar e}{mc} \mathbf{A}(\mathbf{r}) \nabla + iT(\mathbf{r}) \right\} \psi(\mathbf{r}), \quad (4.46)$$

where

$$T(\mathbf{r}) = \frac{1}{2} \int d^3r' \operatorname{Im} K(\mathbf{r}, \mathbf{r} + \mathbf{r}') \sum_{i,k} r'_i r'_k \nabla_i \nabla_k. \quad (4.47)$$

In an isotropic medium, the tensor  $\{1/M(\mathbf{r})\}_{ik}$  is diagonal and  $\mathbf{A}(\mathbf{r}) = 0$ . We note that the concept of an effective mass tensor was introduced in physics by Blokhintsev and Nordheim [52] (also see [51]).

It is useful to clarify the above in terms of solid state physics. For this, we consider the eigenfunctions  $\psi_n(\mathbf{k}, \mathbf{r})$  of an electron in the field of a periodic lattice (here  $n$  is the number of a band):

$$\psi_n(\mathbf{k}, \mathbf{r} + \mathbf{R}_l) = e^{i\mathbf{k}\mathbf{R}_l} \psi_n(\mathbf{k}, \mathbf{r})(\mathbf{k}, \mathbf{r}), \quad \psi_n(\mathbf{k}, \mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} u_n(\mathbf{k}, \mathbf{r}). \quad (4.48)$$

They are called Bloch functions, and the electrons described by them are therefore called Bloch electrons. The form of the Bloch functions indicates the physical sense of the vector  $\mathbf{k}$ : an electron in a crystal can be represented as a plane wave modulated by the lattice period. Studying the general properties of the function  $E_n(k)$  in the neighborhood of selected points in the band  $\mathbf{k}_0$  leads to the relation [15], [51]

$$E_n(\mathbf{k}) = E_n(\mathbf{k}_0) + \frac{\hbar}{m} \mathbf{s} \mathbf{p}_{nn} + \frac{\hbar^2 \mathbf{s}^2}{2m} + \frac{\hbar^2}{m^2} \sum_{j \neq n} \frac{(\mathbf{s} \mathbf{p}_{nj})(\mathbf{s} \mathbf{p}_{jn})}{E_n(\mathbf{k}_0) - E_j(\mathbf{k}_0)} + \dots, \quad (4.49)$$

where the quantities  $\mathbf{p}_{nj}$  and  $\mathbf{s}$  are defined in [15], [51]. This relation shows that the electron described by the Schrödinger equation with a periodic potential can be regarded as a particle affected by an interaction with the potential or as a quasiparticle. The properties of this quasiparticle already include the interaction with the static lattice.

We consider the case where the point  $\mathbf{k}_0$  corresponds to an extremum. For the second derivative of the energy with respect to  $\mathbf{k}$ , we have

$$\frac{m}{\hbar^2} \frac{\partial^2 E_n}{\partial s_\alpha \partial s_\beta} = \frac{m}{\hbar^2} \frac{\partial^2 E_n}{\partial k_\alpha \partial k_\beta} = \delta_{\alpha\beta} + \frac{1}{m} \sum_{j \neq n} \frac{p_{nj}^\alpha p_{jn}^\beta + p_{nj}^\beta p_{jn}^\alpha}{E_n(\mathbf{k}_0) - E_j(\mathbf{k}_0)}. \quad (4.50)$$

Here,  $s_\alpha$  and  $s_\beta$  are the Cartesian coordinates of the vector  $\mathbf{s}$  in some fixed system of axes, and  $p_{nj}^\alpha$  are the corresponding components of the matrix element of the momentum operator. Using the relation

$$\left( \frac{m}{m^*} \right)_{\alpha\beta} = \frac{m}{\hbar^2} \frac{\partial^2 E_n}{\partial k_\alpha \partial k_\beta}, \quad (4.51)$$

we introduce the inverse effective mass tensor. We can then write (4.50) as

$$\left(\frac{m}{m^*}\right)_{\alpha\beta} = \delta_{\alpha\beta} + \frac{1}{m} \sum_{j \neq n} \frac{p_{nj}^\alpha p_{jn}^\beta + p_{nj}^\beta p_{jn}^\alpha}{E_n(\mathbf{k}_0) - E_j(\mathbf{k}_0)}. \quad (4.52)$$

This is often called the sum rule for effective masses and sometimes also called the  $f$ -sum rule. The diagonal elements in (4.52) have a simpler form:

$$\left(\frac{m}{m^*}\right)_{\alpha\alpha} = 1 + \frac{2}{m} \sum_{j \neq n} \frac{|p_{nj}^\alpha|^2}{E_n(\mathbf{k}_0) - E_j(\mathbf{k}_0)}. \quad (4.53)$$

We hence see that the interaction of a given energy level with lower levels or with the states of the ion core, for which  $E_j < E_n$ , leads to a decrease in the effective mass, while interaction with the higher states ( $E_j > E_n$ ) increases it.

The concept of effective mass is well enough defined near either the minimum or maximum of a band. Moreover, the effective mass  $m^*$  near the minimum,

$$E = E_0 + \frac{k_x^2 \hbar^2}{2m^*}, \quad (4.54)$$

differs from the effective mass  $m^{**}$  near the top of the band,

$$E = E_1 + \frac{(k_x - \pi/a)^2 \hbar^2}{2m^{**}}. \quad (4.55)$$

In both cases, the masses  $m^*$  and  $m^{**}$  can significantly differ from the real electron mass. Therefore, if an energy band is very narrow and the curvature of the energy surface near the bottom of the band is small, then the effective mass  $m^*$  is large, sometimes much larger than the real mass. On the other hand, near the top of a band, if the curvature is large, then the mass  $m^{**}$  is very small. The tensor feature of the effective mass (which makes an electron and a hole accelerate differently depending on the field direction) is important for crystals with an asymmetric structure or in the case where the minimum and maximum are not in the center of the Brillouin zone. In some cases, the quantities  $m_x^*$ ,  $m_y^*$ ,  $m_z^*$  must be considered negative; in this case, some of them are positive while others are negative near the saddle point. A close similarity of this mechanism to the theory of the Dirac positron is interesting. A set of systems (e.g., a two-dimensional graphite layer) in which the electron motion is described in terms of relativistic quantum mechanics are currently studied; in these systems, the electron behaves as a zero-mass relativistic particle.

The concept of an effective mass is widespread, especially in the physics of semiconductors and semiconductor devices [15], [51], polaron theory [53], semiconductor superlattices [15], [51], and microelectronics and nanostructure physics [15], [51]. It turned out that the concept of an effective mass is especially useful in conductivity theory and also in other fields of solid state physics, nuclear physics, and so on.

In the theory of systems of many interacting particles, the general concept of quasiparticles [15], which represent the spectrum of elementary excitations of the system with electron–electron, electron–phonon, and other interactions taken into account, is considered. A quasiparticle is a renormalized (dressed in clouds of virtual particles) “seed” (or bare) particle with an effective mass in the form  $m^* = m(1 + \lambda_{e-e} + \lambda_{e-ph})$ . And the renormalized (effective) mass can differ significantly from the original mass, for instance, as in systems of heavy fermions [15].

In some problems in collision theory [15], the concept of an effective mass allows writing a generalized Schrödinger equation with the effective mass  $m^*$  (depending on the particle position) instead of the real

mass  $m$  (this situation is realized in some semiconducting heterostructures). In nuclear physics, using a nonlocal optical potential  $V(\mathbf{r}, \mathbf{r}')$  (under certain conditions) leads to a wave equation for a local potential  $V(\mathbf{r})$  with the effective mass [15]

$$M^*(r) = M \left( 1 - \frac{M\alpha^2}{\hbar^2} V(r) \right)^{-1}. \quad (4.56)$$

In conclusion, we note that the linear Schrödinger-type equation is a sufficiently good approximation for a system of Bose particles under the condition

$$\langle n_\alpha \rangle - |\langle a_\alpha \rangle|^2 = (e^{F_\alpha} - 1)^{-1} \ll 1, \quad (4.57)$$

which in fact agrees with the condition  $\langle n_\alpha \rangle \ll 1$ . This corresponds to involving only weakly excited states in the quasiparticle system. In the case of Fermi statistics, the linear terms cannot be eliminated by shifting operators by a complex number, because this transformation is not canonical. In quantum field theory, the sources (linear in Fermi operators) can be introduced using classical spinor fields anticommuting with both themselves and primary fields. We considered this more complicated case in [54].

We also note that introducing the quantity  $\psi(\mathbf{r})$  does not mean that the state of a small dynamical subsystem becomes a pure state. It remains mixed because it is described by the statistical operator, and the dynamics of the system are described by a system of coupled evolutionary equations for the quantities  $f_\alpha$ ,  $f_\alpha^\dagger$ , and  $F_\alpha$ . There have been numerous attempts to derive a Schrödinger-type equation for a particle in a medium. But it is clear that Eq. (4.38) of the damped Schrödinger equation type is most suitable for describing the dynamical behavior of a particle in a medium in the presence of dissipation. This yields numerous applications of this equation to problems of physics, physical chemistry, biophysics, etc. Various aspects of dissipative behavior and stochastic processes in complicated systems were discussed in detail in [15], [16].

## 5. Damping effects in an open dynamical system

In [55], the applicability of the developed general method to particular problems was shown in an example of calculating the natural width of a spectral line in an atomic system [15]. It is well known that the excited levels in an isolated atomic system, appearing as a result of interaction with its own electromagnetic field, have a finite lifetime. As a result, the levels become quasidiscrete and acquire a finite small width, called the natural width of a spectral line. Consequently, the width of a spectral line equals the inverse lifetime of an excited state.

We consider an atom interacting only with its own electromagnetic field in the approximation of an atom at rest. For simplicity, we assume that the atom can be in only one of two states, the ground and excited states, denoted here by the indices  $\alpha = 1, 2$ , and that the energies  $E_\alpha$  are the relative energies of these states. We thus assume that the atomic system in the excited state plays the role of a small “nonequilibrium” subsystem and the electromagnetic field can be regarded as an analogue of a heat bath. The relaxation (which is the decay of an excited level in this case) occurs via transitions with radiation. We write the Hamiltonian of the complete system as  $H = H_{\text{at}} + H_{\text{f}} + V$ , where

$$H_{\text{at}} = \sum_{\alpha} E_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \quad (5.1)$$

is the Hamiltonian of the atomic subsystem,  $a_{\alpha}^{\dagger}$  and  $a_{\alpha}$  are the creation and annihilation operators for the system in the state  $E_{\alpha}$ , and

$$H_{\text{f}} = \sum_{k,\lambda} kc b_{k,\lambda}^{\dagger} b_{k,\lambda} \quad (5.2)$$



is the Hamiltonian of the transverse electromagnetic field [15], [55], where  $\hbar\mathbf{k}$  is the photon momentum,  $c$  is the speed of light,  $\lambda$  is the polarization index, and  $b_{k,\lambda}^\dagger$  and  $b_{k,\lambda}$  are the creation and annihilation operators for a photon in the state  $(\mathbf{k}\lambda)$ ,  $\lambda = 1, 2$ . The interaction operator  $V$ , which is responsible for transitions with radiation, in the nonrelativistic approximation is

$$V = -\frac{e}{mc}\mathbf{p}\mathbf{A}_{\text{tr}}(\mathbf{r}), \quad (5.3)$$

where  $e$  and  $m$  are the electron charge and mass,  $\mathbf{A}_{\text{tr}}(\mathbf{r})$  is the vector potential (at the point  $\mathbf{r}$ ) of the transverse electromagnetic radiation field, and  $[\mathbf{p} \times \mathbf{A}_{\text{tr}}(\mathbf{r})] = 0$ . The vector potential  $\mathbf{A}_{\text{tr}}(\mathbf{r})$  can be expanded in a series of plane waves:

$$\mathbf{A}_{\text{tr}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{k,\lambda} \left( \frac{2\pi\hbar^2 c}{k} \right)^{1/2} \mathbf{e}_{k,\lambda} (b_{k,\lambda} e^{i\mathbf{k}\mathbf{r}/\hbar} + b_{k,\lambda}^\dagger e^{-i\mathbf{k}\mathbf{r}/\hbar}). \quad (5.4)$$

The  $\mathbf{k}$  sum is over all states of plane waves with the momentum  $\hbar\mathbf{k}$  in a finite box of volume  $\Omega$ . The  $\lambda$  sum is over two allowed directions of photon polarization with the momentum  $\hbar\mathbf{k}$ . The only nonvanishing matrix elements of the creation and annihilation operators  $b_{k,\lambda}^\dagger$  and  $b_{k,\lambda}$  can be represented as

$$\langle n_{k,\lambda} - 1 | b_{k,\lambda} | n_{k,\lambda} \rangle = \sqrt{n_{k,\lambda}}, \quad \langle n_{k,\lambda} + 1 | b_{k,\lambda}^\dagger | n_{k,\lambda} \rangle = \sqrt{n_{k,\lambda} + 1}. \quad (5.5)$$

We now write the interaction operator  $V$  in form (4.9):

$$V = \sum_{\alpha,\beta} \varphi_{\alpha\beta} a_\alpha^\dagger a_\beta, \quad \varphi_{\alpha\beta} = \varphi_{\beta\alpha}^\dagger, \quad (5.6)$$

where

$$\varphi_{\alpha\beta} = \frac{1}{\sqrt{\Omega}} \sum_{k,\lambda} (G_{\alpha,\beta}(k,\lambda) b_{k,\lambda} + b_{k,\lambda}^\dagger G_{\beta\alpha}^*(k,\lambda)), \quad (5.7)$$

$$G_{\alpha,\beta}(k,\lambda) = -\frac{e}{mc} \left( \frac{2\pi\hbar^2 c}{k} \right)^{1/2} \mathbf{e}_{k,\lambda} \langle \alpha | e^{i\mathbf{k}\mathbf{r}/\hbar} \mathbf{p} | \beta \rangle.$$

Here,  $|\alpha\rangle$  and  $|\beta\rangle$  are the eigenvectors of the Hamiltonian  $H_{\text{at}}$  with the eigenvalues  $E_\alpha$  and  $E_\beta$ ,

$$H_{\text{at}}|\alpha\rangle = E_\alpha|\alpha\rangle. \quad (5.8)$$

As usual, we assume that the decay transition of the electric dipole from the state  $a = 1$  to the state  $b = 2$  is permitted, i.e., we consider  $\mathbf{k}\mathbf{r} \ll 1$ . Then  $\varphi_{\alpha\beta}$  becomes

$$\varphi_{\alpha\beta} = -\frac{e}{mc} \langle \alpha | \mathbf{p} | \beta \rangle \sum_{k,\lambda} \left( \frac{2\pi\hbar^2 c}{k} \right)^{1/2} \mathbf{e}_{k,\lambda} (b_{k,\lambda} + b_{k,\lambda}^\dagger). \quad (5.9)$$

The matrix elements of the dipole momentum operator  $\mathbf{d} = e\mathbf{r}$  between the states  $|\alpha\rangle$  and  $|\beta\rangle$  are related to the matrix elements of the momentum  $\mathbf{p}$  as

$$\langle \alpha | \mathbf{p} | \beta \rangle = -\frac{m}{e\hbar} (E_\alpha - E_\beta) \mathbf{d}_{\alpha\beta}. \quad (5.10)$$

Here, we assume that the atom does not have a stationary dipole momentum, i.e.,  $\langle \alpha | \mathbf{p} | \alpha \rangle = 0$ .

We now use the damped Schrödinger-type equation obtained above,

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \sum_\beta K_{\alpha\beta} \langle a_\beta \rangle, \quad (5.11)$$

where

$$K_{\alpha\beta} = \frac{1}{i\hbar} \sum_\gamma \int_{-\infty}^0 dt_1 e^{\varepsilon t_1} \langle \varphi_{\alpha\gamma} \tilde{\varphi}_{\gamma\beta}(t_1) \rangle_{\mathbf{q}}. \quad (5.12)$$

Here,  $\tilde{\varphi}_{\alpha\beta}(t)$  is

$$\tilde{\varphi}_{\alpha\beta}(t) = \varphi_{\alpha\beta}(t) \exp\left(\frac{i}{\hbar}(E_\alpha - E_\beta)t\right). \quad (5.13)$$

It is clear from the above that  $K_{aa} = 0$  and  $K_{ba} = 0$ . We therefore have

$$i\hbar \frac{d\langle a_b \rangle}{dt} = E_b \langle a_b \rangle + K_{bb} \langle a_b \rangle, \quad (5.14)$$

where

$$K_{bb} = \frac{2\pi\hbar^2 e^2}{m^2 c} \frac{1}{\Omega} \sum_k \int_{-\infty}^{\infty} d\omega \frac{1}{k} \frac{J(k, \omega)}{\hbar\omega_0 + \hbar\omega + i\varepsilon} A_{ab}^{ab}\left(\frac{\mathbf{k}}{k}\right), \quad \hbar\omega_0 = E_b - E_a,$$

and we use the notation

$$\begin{aligned} J(k, \omega) &= (\langle n_k \rangle + 1)\delta(\omega + ck) + \langle n_k \rangle \delta(\omega - ck), \\ \langle n_k \rangle &= \sum_\lambda \langle n_{k\lambda} \rangle = (e^{\beta ck} - 1)^{-1} = n(k), \end{aligned} \quad (5.15)$$

and

$$A_{ab}^{ab} = |\langle a|\mathbf{p}|b\rangle|^2 - \left(\langle a|\mathbf{p}|b\rangle \frac{\mathbf{k}}{k}\right) \left(\langle b|\mathbf{p}|a\rangle \frac{\mathbf{k}}{k}\right). \quad (5.16)$$

We then have

$$\begin{aligned} \frac{1}{\Omega} \sum_k \int_{-\infty}^{\infty} d\omega \frac{1}{k} \frac{J(k, \omega)}{\hbar\omega_0 + \hbar\omega + i\varepsilon} A_{ab}^{ab}\left(\frac{\mathbf{k}}{k}\right) &= \\ &= \frac{1}{(2\pi)^3} \int k dk \int_{-\infty}^{\infty} d\omega \frac{1}{k} \frac{J(k, \omega)}{\hbar\omega_0 + \hbar\omega + i\varepsilon} \int d\varpi A_{ab}^{ab}\left(\frac{\mathbf{k}}{k}\right), \end{aligned} \quad (5.17)$$

where  $d\varpi$  is the element of a space angle. We can verify the equality

$$\int d\varpi A_{ab}^{ab}\left(\frac{\mathbf{k}}{k}\right) = \frac{8\pi}{3} |\langle a|\mathbf{p}|b\rangle|^2. \quad (5.18)$$

For the quantity  $K_{bb}$ , we have (here  $\nu = ck$ )

$$K_{bb} = \frac{2e^2}{m^2 c^2 \hbar} |\langle a|\mathbf{p}|b\rangle|^2 \int_0^\infty \nu d\nu \left( \frac{n(\nu) + 1}{\omega_0 - \nu + i\varepsilon} + \frac{n(\nu)}{\omega_0 + \nu + i\varepsilon} \right), \quad (5.19)$$

and we then find the expression for the damping  $\Gamma_b$  at  $T = 0$  K:

$$K_{bb} = \Delta E_b - \frac{i\hbar}{2} \Gamma_b, \quad \Gamma_b = \frac{4}{3} \frac{e^2 \omega_0}{m^2 c^3 \hbar} |\langle a|\mathbf{p}|b\rangle|^2 = \frac{4}{3} \frac{\omega_0^3}{c^3 \hbar} |\mathbf{d}_{ab}|^2. \quad (5.20)$$

This expression coincides with the known value of a natural width of atomic spectral lines [15]. Using the damped Schrödinger-type equation, we can thus simply calculate the energy shift and damping in different particular systems.

It is useful to note that the problem of the natural width of spectral lines has been used many times to test various new calculation schemes and quantum physics theories [15]. For instance, the authors of [56] remarked, “The variety of treatments of the line-broadening problem is so great as to be bewildering, and it is often difficult to see whether different approaches describe, or do not describe, the same effects.” Blokhintsev [57] also considered the problem of the natural width of a spectral line in 1946. In his paper “Calculating spectral line natural width by the stationary method,” he wrote, “The problem of light emission and absorption is usually considered by the method of quantum transitions. Meanwhile, this problem, like the dispersion problem, can be solved extremely simply by the method of stationary states.” Further, the author wrote a system of equations for the amplitudes of states of two types: the emitter is in the state  $m$  without light quanta and the emitter is in the state  $n$  with a single light quantum emitted. Taking the energy conservation law into account, we obtain a solution for the amplitude and an approximate expression based on it for the position of the level of the whole system (emitter and emission). It follows from this expression that we have “exactly the shift and broadened levels that Dirac obtained in calculating the resonance scattering.” Then “the spectral distribution within the width of the line” was found. Blokhintsev noted that in transforming the amplitudes to the coordinate representation, “we obtain a divergent wave whose amplitude increases slowly with increasing distance from the emission source the same as we have for a classical damped oscillator.”

In our approach, we use the concept of “quantum noise.” which allows constructing the NSO with “sources” of noise and obtaining a system of coupled equations for the mean amplitudes and densities as a result. Essentially, the obtained system of equations is analogous (in a certain sense) to the system of Blokhintsev equations for the amplitudes and models the behavior of a “damped oscillator” [57]. The role of friction is played by the interaction  $\varphi_{\alpha\beta}$  of the small system with the medium (heat bath).

## 6. Generalized Van Hove formula

In this section, we briefly consider the problem of scattering slow neutrons in a nonequilibrium medium following [58]. It is known that the microscopic description of the dynamical behavior of condensed matter (gases, fluids, and solids) uses the concept of space–time correlations and the corresponding correlation functions [5], [15], [59]. The slow neutron scattering method [15], [59] is an effective tool for studying the static (structure) and dynamic (quasiparticle excitation spectra) properties of complicated multiparticle systems. The Van Hove theory [15], [59] has a general meaning for describing the scattering of neutrons in a statistical equilibrium state in condensed media. In [15], [59], Van Hove derived the famous formula that allows expressing the scattering cross section for slow neutrons in terms of the Fourier transform of the space–time correlation functions. A generalization of the Van Hove theory to the case of slow neutron scattering on the systems in a nonequilibrium state (e.g., in the presence of gradients of matter, temperature, etc.) was proposed in [58]. The approach described in the preceding sections was used in that case.

We recall, that the basic quantity measured in particle-scattering experiments [15], [59] is the differential scattering cross section. As an example, we first consider a crystal with a lattice constant  $a$ . The transition amplitude for a particle falling on the target is the first-order quantity in the interaction strength between the particle and target. The transition probability from the initial to the final states under the influence of a potential  $V$  can be written as

$$W_{kk'} = \frac{2\pi}{\hbar} \left| \int d^3r \psi_{k'}^* V \psi_k \right|^2 D_{k'}(E'), \quad (6.1)$$

where  $D_{k'}(E')$  is the density of the final states of the scattered particle. We define the cross section as

$$d\sigma = \frac{W_{kk'}}{\text{magnitude of the incident flux}}. \quad (6.2)$$

The incident flux is equal to  $\hbar k'/m$ , and the density of the final states of the scattered particle is

$$D_{k'}(E') = \frac{1}{(2\pi)^3} \frac{d^3 k'}{dE'} = \frac{m^2}{(2\pi)^3 \hbar^3} d\Omega \left( \frac{\hbar k'}{m} \right). \quad (6.3)$$

In this case, we can write the differential scattering cross section as

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi)^2 \hbar^4} \frac{k'}{k} \left| \int d^3 r e^{i(\mathbf{k}' - \mathbf{k})\mathbf{r}/\hbar} V(\mathbf{r}) \right|^2. \quad (6.4)$$

We now use this approach to describe inelastic scattering of slow neutrons [15], [58]. The experiment consists in scattering a monochromatic neutron flux with the energy  $E$  and wave vector  $\mathbf{k}$  on a sample. The scattered neutrons are characterized by the final energy  $E' = E + \hbar\omega$  and direction  $\Omega$  of their final wave vector  $\mathbf{k}'$ . We are interested in the quantity  $I$ , which equals the number of neutrons with wave vectors between  $\mathbf{k}$  and  $\mathbf{k} + d\mathbf{k}$  scattered per unit time:

$$I = I_0 \frac{ma^3}{\hbar k} dw(\mathbf{k} \rightarrow \mathbf{k}') D(\mathbf{k}) d\mathbf{k}, \quad (6.5)$$

where  $m$  is the neutron mass,  $a^3$  is the volume of an elementary target cell,  $dw(\mathbf{k} \rightarrow \mathbf{k}')$  is the transition probability from the initial state  $|\mathbf{k}\rangle$  to the final state  $|\mathbf{k}'\rangle$ , and  $D(\mathbf{k})$  is the state density

$$D(\mathbf{k}) d\mathbf{k} = \frac{a^3}{(2\pi)^3} k^2 d\Omega dk. \quad (6.6)$$

For the wave functions of the incident and scattered particles, we have

$$\psi_{\mathbf{k}} = \sqrt{\frac{m}{k}} e^{i\mathbf{k}\mathbf{r}/\hbar}, \quad \psi_{\mathbf{k}'} = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{k}'\mathbf{r}/\hbar}. \quad (6.7)$$

The transition amplitude for a particle hitting the target is

$$dw(\mathbf{k} \rightarrow \mathbf{k}') = \frac{m}{\hbar^2 k} \frac{d^3 k}{(2\pi\hbar)^3} \int_{-\infty}^{\infty} dt d^3 r d^3 r' \langle V(\mathbf{r}) V(\mathbf{r}', t) \rangle e^{-i(\mathbf{k} - \mathbf{k}')(\mathbf{r} - \mathbf{r}')/\hbar - i\omega t}. \quad (6.8)$$

In other words, we can write the transition amplitude describing the state change of an incident beam per unit time as

$$dw(\mathbf{k} \rightarrow \mathbf{k}') = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dt \text{Tr}(\rho^m V_{\mathbf{k}'\mathbf{k}}(0) V_{\mathbf{k}\mathbf{k}'}(t)) e^{-i\omega t}, \quad (6.9)$$

where  $\rho^m$  is the statistical operator describing the sample (target).

The scattering cross section is

$$\frac{d^2 \sigma}{d\Omega dE'} = \frac{1}{d\Omega d\omega} \frac{I}{I_0} \quad (6.10)$$

or, in a different form,

$$\frac{d^2 \sigma}{d\Omega dE'} = A \int_{-\infty}^{\infty} dt d^3 r d^3 r' \langle V(\mathbf{r}) V(\mathbf{r}', t) \rangle e^{-\frac{i}{\hbar}(\mathbf{k} - \mathbf{k}')(\mathbf{r} - \mathbf{r}') - i\omega t}, \quad (6.11)$$

where

$$A = \frac{m^2}{(2\pi)^3 \hbar^5} \frac{k'}{k}, \quad E' = \frac{(k')^2}{2m}. \quad (6.12)$$

The expression

$$V = \frac{2\pi\hbar^2}{m} \sum_i b_i \delta(\mathbf{r} - \mathbf{R}_i) \quad (6.13)$$

is usually used for the operator of neutron–medium interaction [15], [59]. Here,  $\mathbf{R}_i$  is the position operator for the nucleus of a target atom, and  $b_i$  is the appropriate scattering length. It is also necessary to take into account that

$$V = \sum_{i=1}^N V(\mathbf{r} - \mathbf{R}_i) = \sum_{i=1}^N e^{-i\mathbf{p}\mathbf{R}_i/\hbar} V(\mathbf{r}) e^{i\mathbf{p}\mathbf{R}_i/\hbar} \quad (6.14)$$

and

$$\langle \beta \mathbf{k}' | V | \alpha \mathbf{k} \rangle = \langle \mathbf{k}' | V(\mathbf{r}) | \mathbf{k} \rangle \sum_{i=1}^N \langle \beta | e^{-i\mathbf{k}'\mathbf{R}_i/\hbar} e^{i\mathbf{k}\mathbf{R}_i/\hbar} | \alpha \rangle. \quad (6.15)$$

We hence have

$$\frac{d^2\sigma}{d\Omega dE'} \propto \frac{k'}{k} \frac{1}{2\pi} \sum_{i,j} \int_{-\infty}^{\infty} dt \frac{1}{N} b_i b_j \langle e^{i\kappa\mathbf{R}_i(0)/\hbar} e^{-i\kappa\mathbf{R}_j(t)/\hbar} \rangle e^{-i\omega t}, \quad (6.16)$$

where  $\kappa = k - k'$ . This expression describes the main point of the Van Hove theory [15], [59] that allows writing the inelastic scattering cross section for the slow neutrons in terms of space–time correlations. As mentioned above, in this case, we average with the equilibrium density matrix (statistical operator)  $\rho^m$ , i.e.,  $\langle \bullet \rangle = \text{Tr}(\rho^m \bullet)$ .

We now consider the case of a nonequilibrium medium and use the NSO method. We let  $H_m$  denote the Hamiltonian of the medium (target),  $H_b$  denote the Hamiltonian of the falling neutron beam, and  $V$  denote the interaction operator. The complete Hamiltonian is

$$H = H_0 + V = H_m + H_b + V. \quad (6.17)$$

We write the transition amplitude as

$$dw(\mathbf{k} \rightarrow \mathbf{k}') = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dt \text{Tr}_m(\rho^m(t) V_{\mathbf{k}'\mathbf{k}}(0) V_{\mathbf{k}\mathbf{k}'}(t)) e^{-i\omega t}, \quad (6.18)$$

where  $\rho^m(t)$  is the NSO of the medium (target). In accordance with the above, the scattering cross section is equal to

$$\frac{d^2\sigma}{d\Omega dE'} = A \int_{-\infty}^{\infty} dt d^3r d^3r' \langle V(\mathbf{r}) V(\mathbf{r}', t) \rangle_m e^{-i(\mathbf{k}-\mathbf{k}')(\mathbf{r}-\mathbf{r}')/\hbar - i\omega t}, \quad (6.19)$$

where  $\langle \bullet \rangle_m = \text{Tr}_m(\rho^m(t) \bullet)$  and  $A$  and  $E'$  are defined in (6.12).

We take into the account that

$$\langle \alpha' \mathbf{k}' | V | \alpha \mathbf{k} \rangle = \langle \mathbf{k}' | V(\mathbf{r}) | \mathbf{k} \rangle \sum_{i=1}^N \langle \alpha' | e^{-i(\mathbf{k}'\mathbf{R}_i)/\hbar} e^{i(\mathbf{k}\mathbf{R}_i)/\hbar} | \alpha \rangle. \quad (6.20)$$

As a result, we obtain [15], [58]

$$\begin{aligned} \frac{d^2\sigma}{d\Omega dE'} = & - \frac{1}{(i\hbar)^2} \tilde{A} \sum_{i,j=1}^N \int_0^t d\tau \times \\ & \times \sum_{\alpha} \langle \alpha | \{ e^{i\kappa\mathbf{R}_i(\tau-t)/\hbar} e^{i\kappa\mathbf{R}_j(0)/\hbar} e^{i\omega(\tau-t)} + e^{i\kappa\mathbf{R}_i(0)/\hbar} e^{i\kappa\mathbf{R}_j(\tau-t)/\hbar} e^{-i\omega(\tau-t)} \} \rho^m(t) | \alpha \rangle \end{aligned}$$

or, in another form,

$$\frac{d^2\sigma}{d\Omega dE'} = -\frac{1}{(i\hbar)^2} \tilde{A} \sum_{i,j=1}^N \int_0^t d\tau 2 \operatorname{Re} \langle e^{\frac{i}{\hbar} \boldsymbol{\kappa} \cdot \mathbf{R}_i(\tau-t)} e^{\frac{i}{\hbar} \boldsymbol{\kappa} \cdot \mathbf{R}_j(0)} \rangle_{\text{m}} e^{i\omega(\tau-t)}. \quad (6.21)$$

This expression can be written in terms of the density operator  $n_{\boldsymbol{\kappa}} = \sum_i^N e^{i\boldsymbol{\kappa} \cdot \mathbf{R}_i/\hbar}$  as

$$\frac{d^2\sigma}{d\Omega dE'} = \tilde{A} \cdot 2 \operatorname{Re} \mathcal{S}(\boldsymbol{\kappa}, \omega, t), \quad (6.22)$$

where

$$\mathcal{S}(\boldsymbol{\kappa}, \omega, t) = -\frac{1}{(i\hbar)^2} \int_0^t d\tau e^{i\omega(\tau-t)} \langle n_{\boldsymbol{\kappa}}(\tau-t) n_{-\boldsymbol{\kappa}} \rangle_{\text{m}} \quad (6.23)$$

is called the *scattering function*.

We can write the NSO  $\rho^{\text{m}}(t)$  of the medium (target) as

$$\begin{aligned} \rho^{\text{m}} &= \overline{\rho_{\text{q}}(t,0)} = \varepsilon \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \rho_{\text{q}}(t+\tau, \tau) = \\ &= \varepsilon \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \exp\left(-\frac{H_{\text{m}}\tau}{i\hbar}\right) \rho_{\text{q}}(t+\tau, 0) \exp\left(\frac{H_{\text{m}}\tau}{i\hbar}\right) = \\ &= \varepsilon \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \exp(-S(t+\tau, \tau)). \end{aligned} \quad (6.24)$$

Another form of this expression is

$$\rho^{\text{m}}(t, 0) = \exp(-S(t, 0)) + \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \int_0^t d\tau' \exp(-\tau' S(t+\tau, \tau)) \dot{S}(t+\tau, \tau) \exp(-(\tau'-t)S(t+\tau, \tau)),$$

where

$$\dot{S}(t, \tau) = \exp\left(-\frac{H_{\text{m}}\tau}{i\hbar}\right) \dot{S}(t, 0) \exp\left(\frac{H_{\text{m}}\tau}{i\hbar}\right) \quad (6.25)$$

and

$$\dot{S}(t, 0) = \frac{\partial S(t, 0)}{\partial t} + \frac{1}{i\hbar} [S(t, 0), H] = \sum_m (\dot{P}_m F_m(t) + (P_m - \langle \dot{P}_m \rangle_q^t) \dot{F}_m(t)). \quad (6.26)$$

Finally, the expression for the scattering function of the neutron beam on the nonequilibrium medium is [15], [58]

$$\begin{aligned} \mathcal{S}(\boldsymbol{\kappa}, \omega, t) &= -\frac{1}{(i\hbar)^2} \int_0^t d\tau \langle n_{\boldsymbol{\kappa}}(\tau-t) n_{-\boldsymbol{\kappa}}(0) \rangle_q^t e^{i\omega(\tau-t)} - \\ &= -\frac{1}{(i\hbar)^2} \int_0^t d\tau \int_{-\infty}^0 d\tau' e^{\varepsilon\tau'} (n_{\boldsymbol{\kappa}}(\tau-t) n_{-\boldsymbol{\kappa}}(0), \dot{S}(t+\tau'))^{t+\tau'} e^{i\omega(\tau-1)}. \end{aligned} \quad (6.27)$$

Here,

$$\rho_{\text{q}}(t, 0) = \exp(-S(t, 0)), \quad \langle B \rangle_q^t = \operatorname{Tr}(B \rho_{\text{q}}(t, 0)), \quad (6.28)$$

and we use the standard notation [5]

$$(A, B)^t = \int_0^1 d\tau \operatorname{Tr}[A \exp(-\tau S(t, 0)) (B - \langle B \rangle_q^t) \exp((\tau-1)S(t, 0))]. \quad (6.29)$$

We emphasise that the general feature of the derived expression (6.27) for  $\mathcal{S}(\boldsymbol{\kappa}, \omega, t)$  is the presence of the term  $\dot{S}(t + \tau')$  describing the entropy change. In the case of statistical equilibrium, the entropy change is zero, and only the first term remains in formula (6.27), describing neutron beam scattering in the equilibrium medium.

We note that the problem of neutron scattering in a nonequilibrium medium and of finding the NSO of the medium has many features in common with the problem of describing a small subsystem interacting with a heat bath considered above. In fact, the state of the whole system at the instant  $t$  can be described by a statistical operator of the form

$$\rho(t) = \exp\left(\frac{-iH_0t}{\hbar}\right)\rho(0)\exp\left(\frac{iH_0t}{\hbar}\right), \quad \rho(0) = \rho^m(0) \otimes \rho^b(0). \quad (6.30)$$

The initial state of the medium (target) and of the incident beam of particles implies the factored form of  $\rho(0)$  written as a product of the statistical operator  $\rho^m(0)$  of the medium (target) and the statistical beam operator  $\rho^b(0)$ . At the instant  $t$ , these operators can be written as

$$\begin{aligned} \rho^b(t) &= \text{Tr}_m[\rho(t)] = \text{Tr}_m\left(\exp\left(-\frac{iH_0t}{\hbar}\right)\rho^m(0) \otimes \rho^b(0)\exp\left(\frac{iH_0t}{\hbar}\right)\right), \\ \rho^m(t) &= \text{Tr}_b[\rho(t)] = \text{Tr}_b\left(\exp\left(-\frac{iH_0t}{\hbar}\right)\rho^m(0) \otimes \rho^b(0)\exp\left(\frac{iH_0t}{\hbar}\right)\right), \end{aligned} \quad (6.31)$$

where  $\text{Tr}_m$  and  $\text{Tr}_b$  denote the partial averaging over the respective medium and beam variables.

The general expression for the probability of a transition from the initial state of the statistical system described by the statistical operator  $\rho^i$  to the state with  $\rho^f$  is given by the formula

$$W_{\text{if}}(t) = \text{Tr}(\rho^i(t)\rho^f(t)). \quad (6.32)$$

It is reasonable to assume that  $\rho^i$  can be written in the form  $\rho^i(t) = \rho^i(0) = |k\rangle\langle k|$ . In this case, the transition probability per unit time becomes

$$w_{\text{if}}(t) = \frac{d}{dt} \text{Tr}(|k\rangle\langle k|\rho^f(t)) = \frac{d}{dt} \langle k|\rho^f(t)|k\rangle = \left\langle k \left| \frac{d}{dt} \rho^f(t) \right| k \right\rangle. \quad (6.33)$$

In turn, we can write the generalized Liouville equation (with sources in the right-hand side) for the statistical operator  $\rho(t)$  of the complete system (medium + beam) as

$$\frac{\partial}{\partial t}\rho(t) - \frac{1}{i\hbar}[(H_m + H_b + V), \rho(t)]_- = -\varepsilon(\rho(t) - P\rho(t)), \quad (6.34)$$

where  $P$  is the projection superoperator with the properties

$$P^2 = P, \quad P(1 - P) = 0, \quad P(A + B) = PA + PB. \quad (6.35)$$

The simplest case is

$$P\rho(t) = \rho^{m0} \otimes \rho^b = \rho^{m0} \sum_{\alpha} \langle \alpha | \rho(t) | \alpha \rangle, \quad (6.36)$$

where  $\rho^{m0}$  is the equilibrium statistical operator of the medium.

To describe the nonequilibrium medium, we now use the method of imposing boundary conditions described above. We have

$$\frac{\partial}{\partial t}\rho(t) - \frac{1}{i\hbar}[(H_m + H_b + V), \rho(t)]_- = -\varepsilon(\rho(t) - \rho^m(t)\rho^b(t)), \quad (6.37)$$

where

$$\rho^{\text{m}}(t) = \text{Tr}_{\text{b}} \rho(t) = \sum_k \langle k | \rho(t) | k \rangle \quad (6.38)$$

and (in general case)

$$\rho^{\text{b}} = \text{Tr}_{\text{m}}(\rho(t)) = \sum_{\alpha} \langle \alpha | \rho(t) | \alpha \rangle = \sum_{k,k'} \langle k | \rho^{\text{b}}(t) | k \rangle \langle k' | \alpha \rangle \langle \alpha | k' \rangle = \sum_{k,k'} \rho_{k'k}^{\text{b}} | k \rangle \langle k' |. \quad (6.39)$$

Therefore, according the NSO method, we can rewrite Eq. (6.34) as

$$\frac{\partial}{\partial t} \rho(t) - \frac{1}{i\hbar} [H, \rho(t)]_- = -\varepsilon \left( \rho(t) - \rho^{\text{m}}(t) \sum_q \rho_{qq}^{\text{b}}(t) | q \rangle \langle q | \right), \quad (6.40)$$

where we restrict ourself to diagonal terms of  $\rho^{\text{b}}$  with respect to the states  $|q\rangle$  and where  $\varepsilon \rightarrow 0$  after the thermodynamic limit transition. In this case, the NSO is

$$\begin{aligned} \rho_{\varepsilon} &= \rho_{\varepsilon}(t, 0) = \overline{\rho_{\text{q}}(t, 0)} = \varepsilon \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \rho_{\text{q}}(t + \tau, \tau) = \\ &= \varepsilon \int_{-\infty}^0 d\tau U(\tau) \rho^{\text{m}}(t) \sum_k \rho_{kk}^{\text{b}}(t + \tau) | k \rangle \langle k | U^{\dagger}(\tau), \end{aligned} \quad (6.41)$$

where  $U(t)$  is the evolution operator.

By analogy with the derivation of the evolution equations for a small subsystem interacting with a medium [17], [47], [50], we regard the neutron beam as a small subsystem interacting with a statistical medium in a nonequilibrium state. We can write the appropriate evolution equation in the form

$$\frac{\partial}{\partial t} \rho_{qq}^{\text{b}}(t) = -\frac{1}{i\hbar} \varepsilon \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \sum_k \rho_{kk}^{\text{b}}(t + \tau) \sum_{\alpha} \langle \alpha | \langle q | [U(\tau) \rho^{\text{m}}(t) | k \rangle \langle k | U^{\dagger}(\tau), V]_- | q \rangle | \alpha \rangle. \quad (6.42)$$

Following this analogy, we reasonably restrict ourselves to the lowest-order approximation and assume that memory effects can be disregarded:  $\rho_{kk}^{\text{b}}(t + \tau) \simeq \rho_{kk}^{\text{b}}(t)$ . Integrating by parts, we obtain the evolution equation in the form

$$\frac{\partial}{\partial t} \rho_{qq}^{\text{b}}(t) = \frac{1}{\hbar^2} \sum_k \rho_{kk}^{\text{b}}(t) \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \sum_{\alpha} \langle \alpha | \langle q | [U(\tau) [V(\tau), \rho^{\text{m}}(t) | k \rangle \langle k |]_- U^{\dagger}(\tau), V]_- | q \rangle | \alpha \rangle. \quad (6.43)$$

Just as in deriving the kinetic equations for a system in a heat bath, we restrict ourself to the second order in the interaction  $V$ . It hence follows that we can set  $U = U^{\dagger} = 1$  in Eq. (6.43). As a result, we obtain an equation analogous to Pauli equation (4.24):

$$\frac{\partial}{\partial t} \rho_{kk}^{\text{b}}(t) = \sum_q W_{q \rightarrow k} \rho_{qq}^{\text{b}}(t) - \sum_q W_{k \rightarrow q} \rho_{kk}^{\text{b}}(t). \quad (6.44)$$

Here,  $W_{q \rightarrow k}$  are the effective transition probabilities

$$W_{q \rightarrow k} = 2 \text{Re} \frac{1}{\hbar^2} \int_{-\infty}^0 d\tau e^{\varepsilon\tau} \langle V_{qk} V_{kq}(\tau) \rangle_{\text{m}}^t, \quad (6.45)$$

where  $V_{qk} = \langle q | V | k \rangle$ ,  $\langle \cdot \rangle_{\text{m}}^t = \text{Tr}(\cdot \rho^{\text{m}}(t))$ , and  $\varepsilon \rightarrow 0$  after the thermodynamic limit transition. We thus obtain a generalization of expressions (6.1), (6.9), and (6.17) to the case of a nonequilibrium medium. This directly verifies Eq. (6.23).



## 7. Conclusion

We have briefly analyzed some problems of justifying the NSO method [5] and have shown its flexibility and effectiveness in considering concrete applied problems in nonequilibrium statistical mechanics. In particular, we discussed the derivation of generalized kinetic equations. We generally focused on the problem of the interaction between a small nonequilibrium subsystem and a medium (heat bath). We analyzed its evolution along with the dissipation processes arising as a result of interaction with the medium. Using the NSO method for a dynamical system weakly interacting with a heat bath, we derived a damped Schrödinger-type equation. In this case, we used the auxiliary concept of “quantum noise,” which allowed constructing the NSO with noise “sources” and thus obtaining a system of coupled equations for the mean amplitudes and densities.

As an illustration, we considered the problem of the natural width of spectral lines. This problem arises in considering excited levels in an isolated atomic system that appear with a nonzero probability because of the interaction with its own electromagnetic field and have a finite lifetime. As a result, the levels become quasidiscrete and take a finite small width, called the natural width of a spectral line. We showed that the obtained system of equations is analogous to the system of equations for the state amplitudes and models the behavior of a “damped oscillator.” The role of friction is played by the interaction between the small system and the medium (heat bath). We also obtained a generalized Van Hove formula for the problem of neutron scattering in a nonequilibrium medium. A more detailed and complete discussion of these and other problems of nonequilibrium statistical mechanics can be found in [15], [16], [39]. A further development of the NSO method and its various applications can be found in [5], [14].

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