Irreversible Evolution of Open Systems and the Nonequilibrium Statistical Operator Method

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Abstract

The effective approach to the foundation of the nonequilibrium statistical mechanics on the basis of dynamics was formulated by Bogoliubov in his seminal works. His ideas of reduced description were proved as very powerful and found a broad applicability to quite general time-dependent problems of physics and mechanics. In this paper we analyzed thoroughly the time evolution of open systems in context of the nonequilibrium statistical operator method (NSO). This method extends the statistical method of Gibbs to irreversible processes and incorporates the ideas of reduced description. The purpose of the present study was to elucidate the basic aspects of the NSO method and some few selected approaches to the nonequilibrium statistical mechanics. The suitable procedure of averaging (smoothing) and the notion of irreversibility were discussed in this context. We were focused on the physical consistency of the method as well as on its operational ability to emphasize and address a few important reasons for such a workability.

Key words: Nonequilibrium statistical physics, irreversible processes, method of nonequilibrium statistical operator, equation of evolution, open systems, generalized kinetic equations.

Contents

1 Introduction

As soon as one starts to think about
the nonequilibrium phenomena the questions multiply.
G. Uhlenbeck

The aim of statistical mechanics is to give a consistent formalism for a microscopic description of macroscopic behavior of matter in bulk. Statistical mechanics formulates the consistent approach that successfully describes the stationary macroscopic behavior of many-particle systems as fluids, gases, and solids. It clarifies also the thermodynamic concepts such as heat, temperature, and entropy from the underlying microscopic laws.

It is important to emphasize that in the structure of thermodynamics the one of its basic law, namely the second law, differs very much from other general laws of physics. It is not an equation, but instead states an inequality, which becomes an equality only in the limiting case of a reversible process. There are difficulties with the realization of this limit, because a reversible process is one in which the thermodynamic system never deviates appreciable from equilibrium. However, finite time process involves a disturbance of equilibrium. As a result, it is difficult (if not impossible) to derive the correct equations concerning time rates. It was said sometimes that time appears in thermodynamics not as a quantity but only as the indicator of the sense of a quantity, the change of entropy. The goal of a theory is to describe the actual reality. Real systems are never close. The nonequilibrium statistical thermodynamics aims to describe in the unifying manner irreversible phenomena including nonequilibrium steady states and open systems.

The theoretical study of transport processes in matter is a very broad and well explored field. The methods of equilibrium and nonequilibrium statistical mechanics have been fruitfully applied to a large variety of phenomena and materials. The central problem of nonequilibrium statistical mechanics is to derive a set of equations which describe irreversible processes from the reversible equations of motion. The consistent calculation of transport coefficients is of particular interest because one can get information on the microscopic structure of the condensed matter. There exist a lot of theoretical methods for calculation of transport coefficients as a rule having a fairly restricted range of validity and applicability. The most extensively developed theory of transport processes is that based on the Boltzmann equation. However, this approach has strong restrictions and can reasonably be applied to a strongly rarefied gas of point particles.

During the last decades, a number of schemes have been concerned with a more general and consistent approach to kinetic and transport theory [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. In what follows, we discuss in terse form that direction in the nonequilibrium statistical mechanics which is based on nonequilibrium ensemble formalism and compare it briefly with some other approaches for description of irreversible processes.

These approaches, each in its own way, lead us to substantial advances in the understanding of the nonequilibrium behavior of many-particle classical and quantum systems. This field is very active and there are many aspects to the problem [15, 16, 17, 18]. We survey concisely a formulation of the method of nonequilibrium statistical operator, introduced by Zubarev [5] and some of its applications to concrete problems, with the purpose of making these ideas easier for understanding and applications. The relation to other work is touched on briefly, but the nonequilibrium statistical operator (NSO) method is considered of dominant importance.

2 The Ensemble Method

The formalism of equilibrium statistical mechanics has been developed by Gibbs [19] to describe the properties of many-particle complex physical systems. Central problem in the statistical physics of matter is that of accounting for the observed equilibrium and nonequilibrium properties of fluids and solids from a specification of the component molecular species, knowledge of how the constituent molecules interact, and the nature of their surrounding. It was shown rigorously by Kozlov [20, 21] that the Gibbs canonical distribution (Gibbs ensemble) is the only *universal* one whose density depends on energy and that is compatible with the axioms of thermodynamics.

The ensemble method, as it was formulated by Gibbs [19, 22], have the great generality and the broad applicability to the equilibrium statistical mechanics. The Gibbsian concepts and methods are used today in a number of different fields [15, 16]. Ensembles are a far more satisfactory starting point than *assemblies*, particularly in treating time dependent systems [5, 13, 16]. An ensemble is characterized by the distribution (partition) function $f(\mathbf{p}, \mathbf{q})$ which should satisfy Liouville equation

$$\frac{df}{dt} = 0. \tag{2.1}$$

This purely dynamical requirement reflects the fact that the points in the phase space $(\mathbf{p}, \mathbf{q})$ representing the states of the system in an ensemble do not interact. It is important to realize that the Liouville equation is an expression of the preservation of volumes of phase space.

Equilibrium ensemble theories are rooted in the fundamental principle of equal probability for the microstates of isolated systems [15, 23]. This principle (or postulate) is, in essence, a kind of statistical approximation but mechanical origin.

The notions of the Gibbs state and *Gibbs distribution* [24], which play an important role in determining equilibrium properties of statistical ensembles, were clarified substantially in the last decades. A *Gibbs state* in probability theory and statistical mechanics is an *equilibrium probability distribution* which remains invariant under future evolution of the system.

For systems in the state of statistical equilibrium, there is the Gibbs distribution [19] by means of which it is possible to calculate an average value of any dynamical quantity. No such universal distribution has been formulated for irreversible processes. Thus, to proceed to the solution of problems of statistical mechanics of nonequilibrium systems, it is necessary to resort to various approximate methods. In addition, the Gibbs distributions, have a non-trivial common property: subject to certain constraints it maximize a functional known in statistical mechanics as entropy, and in information theory, probability theory and mathematical statistics as information. The approach based on the information theory in the spirit of the principle of maximum entropy has been used in numerous works on statistical mechanics [5, 15, 25, 26, 27] to derive the fundamental statistical mechanical distributions.

Kubo [15, 18, 28] derived the quantum statistical expressions for transport coefficients such as electric conductivity. This approach considered the case of mechanical disturbances such as an electric field. The mechanical disturbance was expressed as a definite perturbing Hamiltonian and the deviation from equilibrium caused by it can be obtained by perturba-

tion theory. On the other hand, thermal disturbances such as density and temperature gradients cannot be expressed as a perturbing Hamiltonian in an unambiguous way [5, 15, 16]. It is worth noting that there exist a substantial distinction of the standard linear response theory and of the Zubarev's method of the nonequilibrium statistical operator [5, 15, 16]. In essence, the linear response theory is an expansion from the *global* equilibrium state whereas the nonequilibrium statistical operator approach uses the expansion from the *local* (quasi-equilibrium) state. Hence it may provide a more consistent description of various nonequilibrium nonlinear processes.

Temporal evolution of complex statistical systems represents in itself the fundamental aspects of the nonequilibrium statistical physics [1, 2, 3, 4, 5, 6, 7, 15, 16, 28]. It includes also the stochastic nonequilibrium processes [3, 29, 30, 31]. A stochastic process may be considered as the description of a random phenomenon evolving in time that is governed by certain laws of probability. To describe these complicated behaviors various generalized statistical mechanics methods for complex systems were developed [1, 2, 3, 4, 5, 6, 7, 15, 16, 28, 29, 30, 31]. The answers on a question of how to obtain an irreversible description of temporal processes are numerous [5, 6, 7, 15, 32]. Usually the statistical-mechanical theory of transport is divided into two related problems: the mechanism of the approach to equilibrium, and the representation of the microscopic properties in terms of the macroscopic fluxes.

It is well known [5] that in a standard thermodynamic approach one deals with only a small number of state variables to determine the properties of a uniform equilibrium system. To deal with irreversible processes in systems not too far from equilibrium, one divides the system into small subsystems and assumes that each subsystem is in *local equilibrium* [5, 15, 16], i.e., it can be treated as an individual thermodynamic system characterized by the small number of physical variables. For continuous systems, there is a temperature T associated with each subsystem, and $T\sigma$ is the *dissipation*; here σ is the "entropy production", which is defined as the time rate of the entropy created internally by an irreversible process [33, 34, 35]. Note, that according to the law of thermodynamics, reversible evolution is an evolution with constant entropy.

If $T\sigma$ is calculated for various irreversible processes, it is always found to have the form

$$T\sigma = \sum_i J_i X_i > 0,$$

where J_i are flows of the matter, heat, etc., and X_i are generalized driving forces for vector transport processes or for chemical reactions, etc. The J_i and X_i are linearly related when the system is not too far from equilibrium. Thus

$$J_i = \sum_i L_{ij} X_j,$$

where the L_{ij} are called phenomenological transport coefficients. The aim of the nonequilibrium statistical mechanics is to calculate these transport coefficients microscopically.

Great efforts have been directed by numerous authors toward establishing the theory of irreversible processes on a microscopic basis [5, 15, 16]. Zwanzig [36] have reformulated the methods of Prigogine and Van Hove. His reformulation was characterized by extensive use of Gibbsian ensembles. Projection operators in the space of all possible ensemble densities were used to separate an ensemble density into a *relevant* part, required for the calculation

of ensemble averages of specified quantities, and the remaining *irrelevant* part. This was a generalization of the common separation of a density matrix into diagonal and nondiagonal parts, as used in derivation of the master equation.

Zwanzig showed that the Liouville equation is the natural starting point for a theory of time-dependent processes in statistical mechanics. He considered the ensemble density (phase space distribution function or density matrix) $f(t)$ at time t. The average of a dynamical variable A (function, matrix or operator) at time t is $\langle A; f(t) \rangle$. Thus, the main tool in Zwanzig reformulation [8, 9, 11, 36] was the use of projection operators in the Hilbert space of Gibbsian ensemble densities. Projection operators are a convenient tool for the separation an ensemble density into a *relevant* part, needed for the calculation of mean values of specified observables, and the remaining *irrelevant* part. The *relevant* part was shown to satisfy a kinetic equation which is a generalization of Van Hove master equation; diagram summation methods were not used in this approach.

Hence, the Gibbs ensemble in statistical mechanics serves as a microscopic formulation of equilibrium thermodynamics, and the fluctuation-dissipation theorem provides a microscopic connection to the system response functions and transport coefficients which characterize small departures from equilibrium. Far from equilibrium, Lyapunov expansion is a property with the potential to provide a useful microscopic description, when local definitions of quasi-equilibrium quantities, such as temperature and pressure, may no longer have meaning. The Lyapunov exponent measures the rate at which a system "forgets" its initial conditions. The transport coefficients are those response functions of the system that also measure a "forgetting". For example, scattering erases a particle's memory of its original velocity and so give rise to a finite diffusion coefficient. Many authors have been exploring the connection between transport coefficients and Lyapunov exponents [15, 16].

3 Bogoliubov's Fundamental Results

Bogoliubov contributed greatly to equilibrium and nonequilibrium statistical mechanics and received many fundamental results. The intense current interest in the statistical mechanics of irreversibility is in the foundation of the nonequilibrium statistical mechanics on the basis of dynamics. The important contribution of Bogoliubov are his notable papers on dynamical theory and physical kinetics [1, 2, 3]. There he introduced the key concept of the hierarchy of relaxation times in statistical physics. This method relies substantially on the existence of the natural fine-scale mixing occurring in dynamics.

Bogoliubov method emphasized three important points: (i) Temporal Evolution; (ii) Reduced Description (Relevant Variables);(iii) Averaging Procedure. These ideas have a fundamental role in the description of multi-scale systems characterized by hierarchical configurations of complex many-particle systems.

Bogoliubov approach leads to a systematic development of the equations describing the time evolution of the two-particle, three-particle, etc., distribution functions, and treats the time development as occurring in rather well-defined stages. At each stage the system has "*forgotten*" more and more of the information contained in the initial n-particle distribution function. Thus Bogoliubov assumed that after a time of the order of the duration of a collision between molecules, all the higher-order distribution functions will depend on time only as functionals of the single-particle distribution function. At the next, or "hy-

drodynamic" stage, only the first few moments of the single-particle distribution function, i.e., the local values of density, temperature, and flow velocities, are needed to describe the evolution of the system.

A method of obtaining a system of coupled equations for the probability densities for groups of one or more particles was proposed. This has proved to be the most effective method in statistical mechanics for equilibrium and non-equilibrium systems to date. In his approach Bogoliubov clarified how stochastic behavior, which is specific for a macroscopic description, arises in a purely mechanistic approach, in which microscopic equations of dynamical theory are used.

Bogoliubov introduced the concept of stages of the evolution - chaotic, kinetic, and hydrodynamic and the notion of the time scales, namely, interaction time τ_{coll}, free path time τ_{fp}, and time of macroscopic relaxation τ_{rel}, which characterize these stages, respectively. At the chaotic stage, the particles synchronize, and the system passes to a *local equilibrium*. At the kinetic stage, all distribution functions begin to depend on time via the one-particle function. Finally, at the hydrodynamic stage, the distribution functions depend on time via macroscopic variables, and the system approaches equilibrium.

For dilute gas, when the time of intermolecular interaction (interaction time, τ_{coll}) is less than the free path time, there are two kinds of processes: *fast* and *slow*. Hence for the fast processes characteristic time is of the order τ_{coll} and for slow processes - of the order τ_{fp}.

Moreover, Bogoliubov for the first time formulated the *boundary conditions* for the chain of the n-particle distribution functions. These conditions correspond to the *reduced description* and replace the Boltzmann's hypothesis of the *molecular chaos*. Indeed, in the Boltzmann approach the irreversibility feature was connected with the assumption that information about individual molecular dynamics is forgotten after the collisions (for rarefied gas). In contrast, only the probability distribution of velocities among the particles was remembered. Hence, this lack of memory (or continual randomization) namely may be considered as the real source of irreversibility. As it was showed clearly by Bogoliubov, the system should be *large enough* in order to the randomization assumption was reasonably applicable.

In this connection, a significant contribution in the rigorous treatment of the thermodynamic limit [27] was made by Bogoliubov, who developed a general formalism for establishing of the limiting distribution functions in the form of formal series powers of the density. Bogoliubov outlined the method of justification of the thermodynamic limit and derived the generalized Boltzmann equations from his formalism. Bogoliubov also introduced the important clustering principle. Bogoliubov conjectured that it is often convenient to separate the dependence on momenta and consider distribution functions, which will depend only on coordinates passing then to the thermodynamic limit. Thus, on the basis of his equations for distribution functions and the cluster property, the Boltzmann equation was first obtained without employing the molecular chaos hypothesis.

4   Nonequilibrium Ensembles

Here, we remind very briefly the main streams of the nonequilibrium ensembles approaches to statistical mechanics. Beginning have been made by Lebowitz and Bergmann [37, 38, 39, 40] and some other authors.

The central statement of the statistical-mechanical picture is the fact that it is practically impossible to give a complete description of the state of a complex macroscopic system. We must substantially reduce the number of variables and confine ourselves to the description of the system which is considerably less then complete. The problem of predicting probable behavior of a system at some specified time is a statistical one [1, 2, 3, 5]. It is useful and workable to employ the technique of representing the system by means of an ensemble [19] consisting of a large number of identical copies of a single system under consideration. The state of ensemble is then described by a distribution function $\rho(\mathbf{r}_1 \ldots \mathbf{r}_n, \mathbf{p}_1 \ldots \mathbf{p}_n, t)$ in the phase space of a single system. This distribution function is chosen so that averages over the ensemble are in exact agreement with the incomplete (macroscopic) knowledge of the state of the system at some specified time. Then the expected development of the system at subsequent times is modelled via the average behavior of members of the representative ensemble. It is evident that there are many different ways in which an ensemble could be constructed. As a result, the basic notion, the distribution function ρ is not uniquely defined. Moreover, contrary to the description of a system in the state of thermodynamic equilibrium which is only one for fixed values of volume, energy, particle number, etc., the number of nonequilibrium states is large.

The precise definition of the nonequilibrium state is quite difficult and complicated task, because of this state is not specified uniquely. However in certain cases the thorough considerations lead to the establishment of various time scales [1, 2, 3, 5]. In fact, the quasi-equilibrium and nonequilibrium formulations are quite similar in structure and functional dependence. Thus, a large and important class of transport processes can reasonably be modelled in terms of a reduced number of macroscopic *relevant variables* [5].

This line of reasoning has led to seminal ideas on the construction of Gibbs-type ensembles for nonequilibrium systems. Such a program is essentially designed to develop a statistical-mechanical description of nonequilibrium processes, motivated by the success of the statistical mechanics of Gibbs for the equilibrium state. The possibility of carrying over Gibbs approach to nonequilibrium statistical mechanics was anticipated by Callen and Welton [41] in connection with the fluctuation-dissipation theorem [5].

In attempting to develop such a theory it must be kept in mind that in order for a system to approach s steady state, or to remain in a nonequilibrium stationary state, it cannot be isolated but must be in contact with surroundings (reservoirs) which maintain gradients within it.

The attempt to construct general nonequilibrium ensembles was carried out by Lebowitz and Bergmann [37, 38, 39, 40]. They used a model reservoir that, as far as the system was concerned, always had the same appearance and consisted of an infinite number of independent, identical components, each of which interacted with the system but once. Thus the process can be considered as the truly stationary. They assumed also that there was an impulsive interaction between system and reservoir components. So, it was not necessary to deal with the total, infinite, phase-space of the reservoir. In this approach these reservoirs played the role of thermodynamic temperature baths. The ensemble, representing a system in contact with such reservoirs, obeys an integro-differential equation in Γ-space, containing both the Liouville equation and a stochastic integral term that describes the collision with the reservoirs. The Onsager relations [5, 16] were obtained without any reference to fluctuation theory and without the assumption of detailed balancing. They derived the stationary distribution (via an iteration procedure). Lebowitz [39] has found exact

stationary nonequilibrium solutions for some simple systems, and has introduced a simple relaxation-type method for finding approximate stationary solutions for the distribution function. This program was not fully successful. The difficult aspect of this approach was in the handling in detail the interaction between the system and reservoir, making its utility uneasy.

A method similar to the method of nonequilibrium statstical operator [5] was formulated by McLennan [6]. His method is based on the introduction of external forces of a non-conservative nature, which describe the influence of the surroundings or of a thermal bath on the given system. In other words, McLennan operates with the energy and particle reservoirs and movable pistons in contact with the system. The evolution equation for the distribution function f_U within the McLennan approach has the following form

$$\frac{\partial f}{\partial t} + [f, H] + \frac{\partial f F_\alpha}{\partial p_\alpha} = 0, \tag{4.1}$$

where

$$F_\alpha = -\int gX \frac{\partial U}{\partial q_\alpha} d\Gamma_s. \tag{4.2}$$

Here U is the Hamiltonian of the interaction with the surroundings, $f = \int f_U d\Gamma_s$, $g = \int f_U d\Gamma$, $f_U = fgX$, q_α and p_α are the coordinates and momenta of the system. The quantity F_α has the meaning of a "*force*" representing the action of the surrounding on the system (for details see Refs. [5, 6, 15]).

Nevertheless, it was become clear that the sophisticated ideas are required for describing a situation when we need to average over reversible dynamical equations and acquire the irreversible equations; the numerous approaches for solution of this problem were proposed. The essence of the task was summarized by Mayer [42]: "The properties of a macroscopic classical system consisting of some 10^{23} molecules are determined by a probability density function W of the complete Γ space of moments and coordinates of all the molecules. This probability density function is that of the ensemble representing the totality of all experimental systems prepared according to the macroscopic specifications. The entropy is always to be defined as the negative of k_B times the integral over the distinguishable phase space of $W\ln W$. However, the total probability density function W, even for a thermodynamically isolated system, does not obey the Liouville equation, $\partial W/\partial t = LW$, since small fluctuations due to its contact with the rest of the universe necessarily "smoothes" W, by smoothing the direct many-body correlations in its logarithm. This smoothing is the cause of the entropy increase, and in systems near room temperature and above, in which there is heat conduction or chemical species diffusion, the smoothing keeps the true entropy numerically equal to that inferred from the local temperatures, pressures, and compositions. This, however, is by no means necessarily general. The criterion of thermodynamic isolation is not that the complete probability density function W is unaffected by the surroundings, but that reduced probability density functions w_n in the Γ space of $n = 2, 3, \ldots$ molecules evolve in time as if the system were unaffected by the surroundings. This criterion is sufficient to give a mathematically definable method of "smoothing" the complete probability density function. The smoothing consists of replacing the direct many-body correlations in $\ln W$ by their average n-body values, $n = 2, 3, \ldots$, such that the smaller reduced probability density functions w_n are unaffected".

Method of averaging in complex many-particle (nonlinear) systems was elaborated by

Bogoliubov, Krylov and Mitropolski. It was discussed and generalized by various authors [43, 44, 45, 46]. In this context, it was shown by Bogoliubov [47] that the mixing property arising in ergodic theory is not necessary for statistical systems for *any finite* volume and number of particles. Of importance is only the appropriate behavior of the *limiting average values* of the macroscopic quantities at $t \to \infty$ after the transition to the limit of statistical mechanics [48] has been performed.

Bogoliubov emphasizes [47] the fact that ergodic theory in its standard form is not sufficiently established. In order to explain this idea, some model systems were investigated, i.e. the problem of interaction of the particle with quantum field. The open mathematical questions in this field were pointed and it was especially stressed that one has not succeeded yet in rigorous proving the properties of many-particle systems which were required by the basic postulate of statistical mechanics. These conclusions by Bogoliubov [47] anticipated the subsequent critical arguments [49] by Earman and Redei and other authors "why ergodic theory does not explain the success of equilibrium statistical mechanics". It is worth noting that relatively recently a certain progress in this field was achieved in the remarkable publications [50, 51], where generalizations of the classical Birkhoff and von Neumann ergodic theorems were presented. The time average with the aid of special summation methods was replaced by a more general average, including some density ϱ. The character of averaging differs fundamentally from classical uniform averaging.

The main theoretical aspects of the problem of averaging were clarified by Bogoliubov in his seminal works. He formulated the proper method of "*averaging*" and carried out a full mathematical justification of it. This line of reasoning was refined and developed further by Bogoliubov and Mitropolsky [43, 44]. They have elaborated perturbation methods to obtain asymptotic solutions without secular terms. In this approach [43, 44], the main intention was to find a transformation of variables which would separate the "*slow*" variables from the "*fast*" ones. Subsequently, Bogoliubov worked out a rigorous theory of the averaging method and showed that it is naturally related to the existence of a certain transformation of variables that enables one to eliminate the time t from the right-hand sides of the corresponding equations to within an arbitrary accuracy relative to the small parameter ε. At the same time, invoking subtle physical considerations, he showed how to construct not only the first-approximation system (averaged system), but also averaged systems in higher approximations, whose solutions approximate the solutions of the original (exact) system to within an arbitrary prescribed accuracy [43, 44, 45, 46].

A brilliant example of the physical problem where separation of the "*slow*" variables a from the "*fast*" ones ψ within Krylov-Bogoliubov method was especially successful, was the work of Bogoliubov and Zubarev [52] on plasma in the magnetic field. It was shown later how this method can be generalized to higher order of the perturbation expansion in the case of nearly periodic or nearly quasi-periodic systems.

In the present context, it is of importance to stress that the averaging method in the nonlinear mechanics [43] has much in common with the statistical mechanics [5, 46]. These ideas were implemented ingeniously by Zubarev [5] in his NSO method. Indeed, there is a close analogy with the statistical mechanical problematic. In other words, in both the equilibrium and nonequilibrium statistical mechanics the real relevant variables of interest are the properly *averaged* (or time-smoothed) set of variables.

5 The Method of Nonequilibrium Statistical Operator

The method of nonequilibrium statistical operator (NSO) developed by Zubarev [5] is the satisfactory and workable approach to construction of Gibbs-type ensembles for nonequilibrium systems. The NSO method permits one to generalize the Gibbs ensemble method to the nonequilibrium case naturally, and to construct a nonequilibrium statistical operator which enables one to obtain the transport equations and calculate the kinetic coefficients in terms of correlation functions, and which, in the case of equilibrium, goes over to the Gibbs distribution.

The NSO method sets out as follows. The irreversible processes which can be considered as a reaction of a system on mechanical perturbations can be analyzed by means of the method of linear reaction on the external perturbation [5, 15, 16]. However, there is also a class of irreversible processes induced by thermal perturbations due to the internal inhomogeneity of a system. Among them we have, e.g., diffusion, thermal conductivity, and viscosity. In certain approximate schemes it is possible to express such processes by mechanical perturbations which artificially induce similar nonequilibrium processes. However, the fact is that the division of perturbations into mechanical and thermal ones is reasonable in the linear approximation only [15]. In the higher approximations in the perturbation, mechanical perturbations can lead effectively to the appearance of thermal perturbations. The NSO method permits one to formulate a workable scheme for description of the statistical mechanics of irreversible processes which includes the thermal perturbation in a unified and coherent fashion. To perform this, it is necessary to construct statistical ensembles representing the macroscopic conditions determining the system. Such a formulation is quite reasonable if we consider our system for a suitable large time. For these large times the particular properties of the initial state of the system are irrelevant and the relevant number of variables necessary for description of the system reduces substantially.

A central issue in the statistical thermodynamics is the quest for the state functions that describe the changes of all relevant (measurable) equilibrium quantities in terms of a set suitable state variables (thermodynamic state variables), that is, a set of variables that uniquely determine a thermodynamic state. Equilibrium thermodynamics is based on two laws, each of which identifies such a state functions. For the nonequilibrium thermodynamics the problem of a suitable choice of the relevant variables is much more complicated.

The assumption of *local equilibrium* is a basic and necessary assumption in linear irreversible thermodynamics [5, 15, 16, 28, 32]. It enables us to apply the equations of equilibrium thermodynamics, such as the Gibbs equation, to local volume elements in a system. The entropy and other thermodynamic properties of the system can then be defined in terms of local, intensive state variables. The assumption leads to the concept of an *entropy production* in a system subject to irreversible processes [5, 28, 33, 34, 35, 53, 54].

Validity conditions for partial and complete local thermodynamic equilibrium in many-particle system play an important role in the field of equilibrium and nonequlibrium statistical mechanics. A physical system is in an *equilibrium state* if all currents - of heat, momentum, etc., - vanish, and the system is uniquely described by a set of state variables, which do not change with time.

From a general point of view, all laws and thermodynamic relations for complete thermodynamic equilibrium also hold in the case of complete local thermodynamic equilibrium. However, the only exception from this rule makes Planck radiation law [55, 56, 57, 58]. In

connection with the foundations of statistical mechanics, the relations between thermodynamics and dynamics was considered in the context of the fact that in quantum mechanics, equipartition should be replaced by Planck's law [55, 56, 57, 58].

But even in those cases in which complete local thermodynamic equilibrium does not further exist, partial local thermodynamic equilibrium (quasi-equilibrium) may still be realized, thus, permitting nevertheless useful applications of general thermodynamic formulas under restricted conditions.

A case of considerable practical interest in connection with the phenomena of nonequilibrium processes is that of the *hierarchy of time scales*. One of the essential virtues of the NSO method is that it focuses attention, at the outset, on the existence of different time scales. Suppose that the Hamiltonian of our system can be divided as $H = H_0 + V$, where H_0 is the dominant part, and V is a weak perturbation. The separation of the Hamiltonian into H_0 and V is not unique and depends on the physical properties of the system under consideration. The choice of the operator H_0 determines a short time scale τ_0. This choice is such that for times $t \gg \tau_0$ the nonequilibrium state of the system can be described with a reasonable accuracy by the average values of some finite set of the operators P_m.

After the short time τ_0, it is supposed that the system can achieve the state of an incomplete or quasi-equilibrium state. The main assumption about the quasi-equilibrium state is that it is determined completely by the quasi-integrals of motion which are the internal parameters of the system. The characteristic relaxation time of these internal parameters is much longer than τ_0. Clearly then, that even if these quasi-integrals at the initial moment had no definitive equilibrium values, after the time τ_0, at the quasi-equilibrium state, those parameters which altered quickly became the functions of the external parameters and of the *quasi-integrals of motion*. It is essential that this functional connection does not depend on the initial values of the parameters. In other words, the operators P_m are chosen so that they should satisfy the condition

$$[P_k, H_0] = \sum_l c_{kl} P_l. \tag{5.1}$$

It is necessary to write down the transport equations for this set of *relevant* operators only. The relevant operators may be scalars or vectors. The equations of motion for the average of other *irrelevant* operators (other physical variables) will be in some sense consequences of these transport equations. As for the *irrelevant* operators which do not belong to the reduced set of the *relevant* operators P_m, relation (5.1) leads to the infinite chain of operator equalities. For times $t \leq \tau_0$ the nonequilibrium averages of these operators oscillate fast, while for times $t > \tau_0$ they become functions of the average values of the operators.

To carry out into practice the statistical thermodynamics of irreversible processes so that thermal perturbations were included, it is necessary to construct a statistical ensemble representing the macroscopic conditions for the system [5]. For the construction of a nonequilibrium statistical operator [5] the basic hypothesis is that after small time-interval τ the nonequilibrium distribution is established. Moreover, it is supposed that it is weakly time-dependent by means of its parameter only. Then the statistical operator ρ for $t \geq \tau$ can be considered as an *integral of motion* of the quantum Liouville equation

$$\frac{\partial \rho}{\partial t} + \frac{1}{i\hbar}[\rho, H] = 0. \tag{5.2}$$

Here $\partial\rho/\partial t$ denotes time differentiation with respect to the time variable on which the relevant parameters F_m depend. It is important to note once again that ρ depends on t by means of $F_m(t)$ only. These parameters are given through the external conditions for our system and, therefore, the term $\partial\rho/\partial t$ is the result of the external influence upon the system; this influence causes that the system is non-stationary. In other words we may consider that the system is in thermal, material, and mechanical contact with a combination of thermal baths and reservoirs maintaining the given distribution of parameters F_m. For example, it can be the densities of energy, momentum, and particle number for the system which is macroscopically defined by given fields of temperature, chemical potential and velocity. It is assumed that the chosen set of parameters is sufficient to characterize macroscopically the state of the system. Thus the choice of the set of the relevant parameters are dictated by the external conditions for the system under consideration.

In order to describe the nonequilibrium process, it is supposed that the reduced set of variables incoming into ρ is chosen as the average value of some reduced set of relevant operators P_m, where m is the index (continuous or discrete). For the suitable choice of operators P_m such approach is possible for hydrodynamic and kinetic stage of the irreversible process.

The equations of motions for P_m will lead to the suitable *evolution equations* [5]. In the quantum case we have:

$$\frac{\partial P_m(t)}{\partial t} - \frac{1}{i\hbar}[P_m(t), H] = 0. \tag{5.3}$$

The time argument of the operators $P_m(t)$ denotes the Heisenberg representation with the Hamiltonian H independent of time. Then we suppose that the state of the ensemble is described by a nonequilibrium statistical operator which is a functional of $P_m(t)$

$$\rho(t) = \rho\{\ldots P_m(t)\ldots\}. \tag{5.4}$$

For the description of the hydrodynamic stage of the irreversible process the energy, momentum and number of particles densities, $H(x)$, $\mathbf{p}(x)$, $n_i(x)$ should be chosen as the operators $P_m(t)$. For the description of the kinetic stage the occupation number of one-particle states can be chosen. It is necessary to take into account that $\rho(t)$ satisfies the Liouville equation. Hence the quasi-equilibrium (local-equilibrium) Gibbs-type distribution will have the form

$$\rho_q = Q_q^{-1} \exp\left(-\sum_m F_m(t)P_m\right), \tag{5.5}$$

where the parameters $F_m(t)$ have the sense of time-dependent thermodynamic parameters, e.g., of temperature, chemical potential, and velocity (for the hydrodynamic stage), or the occupation numbers of one-particle states (for the kinetic stage). The statistical functional Q_q is defined by demanding that the operator ρ_q be normalized and equal to

$$Q_q = \mathrm{Tr}\exp\left(-\sum_m F_m(t)P_m\right). \tag{5.6}$$

In addition, it was shown that there exists general method for choosing a suitable quasi-equilibrium distribution [5]. For the state with the extremal value of the *informational entropy* [5, 15, 25, 26, 27, 54]

$$S = -\mathrm{Tr}(\rho\ln\rho), \tag{5.7}$$

provided that

$$\mathrm{Tr}(\rho P_m) = \langle P_m \rangle_q; \quad \mathrm{Tr}\rho = 1, \tag{5.8}$$

it is possible to construct a suitable quasi-equilibrium ensemble [59, 60, 61]. Here the notation used is $\langle \ldots \rangle_q = \mathrm{Tr}(\rho_q \ldots)$. Then the corresponding quasi-equilibrium (or local equilibrium) distribution has the form [59, 60, 61]

$$\rho_q = \exp\left(\Omega - \sum_m F_m(t)P_m\right) \equiv \exp(-S(t,0)), \quad \Omega = \ln \mathrm{Tr}\exp\left(-\sum_m F_m(t)P_m\right), \tag{5.9}$$

where $S(t,0)$ can be called the entropy operator. Indeed, the conditional extremum [59, 60, 61] of the functional (5.7) corresponds to the extremum of

$$\Phi(\rho) = -\mathrm{Tr}(\rho \ln \rho) - \sum_m F_m \mathrm{Tr}(\rho P_m) + \lambda \mathrm{Tr}\rho, \tag{5.10}$$

where $F_m(t)$ and λ denote Lagrange multipliers. From the condition

$$\delta \Phi(\rho) = 0, \tag{5.11}$$

we find the expression for ρ_q.

The quasi-equilibrium statistical operator preserves the thermodynamic formulae for the parameters $F_m(t)$

$$\frac{\delta \Phi}{\delta F_m} = -\langle P_m \rangle_q, \tag{5.12}$$

but the Liouville equation is not satisfied.

In other words, the form of the quasi-equilibrium statistical operator was constructed in such a way that to ensure that the thermodynamic equalities for the relevant parameters $F_m(t)$

$$\frac{\delta \ln Q_q}{\delta F_m(t)} = \frac{\delta \Omega}{\delta F_m(t)} = -\langle P_m \rangle_q; \quad \frac{\delta S}{\delta \langle P_m \rangle_q} = F_m(t) \tag{5.13}$$

are satisfied. It is clear that the variables $F_m(t)$ and $\langle P_m \rangle_q$ are thermodynamically conjugate. Since that the operator ρ_q itself does not satisfy the Liouville equation, it should be modified [5] in such a way that the resulting statistical operator satisfies the Liouville equation. This is the most delicate and subtle point of the whole method. To clarify this point let us modify the quasi-equilibrium operator such that the Liouville equation would be satisfied with the accuracy up to $\varepsilon \to 0$. If we shall simply look for the statistical operator, which in a some initial moment is equal to the quasi-equilibrium operator, then, if the initial moment is fixed, we will have the transition effects for small time intervals. These effects has not any real physical meaning. This is why Zubarev [5] used another way, remembering the averaging method in the nonlinear mechanics, which has much in common with the statistical mechanics. As it was pointed above, if the nonlinear system tends to the limiting cycle it "*forget*" about the initial conditions, as well as in the statistical mechanics. Thus, according to Zubarev, the suitable variables (*relevant operators*), which are time-dependent by means of $F_m(t)$, should be constructed by means of taking the *invariant part* of the operators incoming into the logarithm of the statistical operator with respect to the motion with Hamiltonian H. Thus, by definition a special set of operators should

be constructed which depends on the time through the parameters $F_m(t)$ by taking the *invariant part* of the operators $F_m(t)P_m$ occurring in the logarithm of the quasi-equilibrium distribution, i.e.,

$$B_m(t) = \overline{F_m(t)P_m} = \varepsilon \int_{-\infty}^{0} e^{\varepsilon t_1} F_m(t+t_1)P_m(t_1)dt_1 = \tag{5.14}$$

$$F_m(t)P_m - \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \left(F_m(t+t_1)\dot{P}_m(t_1) + \dot{F}_m(t+t_1)P_m(t_1) \right),$$

where $(\varepsilon \to 0)$ and

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

The parameter $\varepsilon > 0$ will be set equal to zero, but only *after the thermodynamic limit* [23] has been taken. Thus, the invariant part is taken with respect to the motion with Hamiltonian H. The operators $B_m(t)$ satisfy the Liouville equation in the limit $(\varepsilon \to 0)$

$$\frac{\partial B_m}{\partial t} - \frac{1}{i\hbar}[B_m, H] = \varepsilon \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \left(F_m(t+t_1)\dot{P}_m(t_1) + \dot{F}_m(t+t_1)P_m(t_1) \right). \tag{5.15}$$

The operation of taking the invariant part, or *smoothing* the oscillating terms, is used in the formal theory of scattering to set the boundary conditions which exclude the advanced solutions of the Schrödinger equation [5, 15]. It is most clearly seen when the parameters $F_m(t)$ are independent of time. Differentiating $\overline{P_m}$ with respect to time gives

$$\frac{\partial \overline{P_m(t)}}{\partial t} = \varepsilon \int_{-\infty}^{0} e^{\varepsilon t_1} \dot{P}_m(t+t_1)dt_1. \tag{5.16}$$

The $\overline{P_m(t)}$ can be called the integrals (or *quasi-integrals*) of motion, although they are conserved only in the limit $(\varepsilon \to 0)$. It is clear that for the Schrödinger equation such a procedure excludes the advanced solutions by choosing the initial conditions. In the present context this procedure leads to the selection of the retarded solutions of the Liouville equation.

The choice of the exponent in the statistical operator can be confirmed by considering its extremum properties [5, 59, 60, 61]. The requirement is that the statistical operator should satisfy the condition of the minimum of the information entropy provided that

$$\langle P_m(t_1) \rangle^{t+t_1} = \text{Tr}(\rho_q P_m(t_1))); \quad \text{Tr}\rho_q = 1, \tag{5.17}$$

in the interval $(-\infty \le t_1 \le 0)$, i.e. for all moments of the past and with the preserved normalization. To this conditional extremum corresponds the extremum of the functional [5, 59, 60, 61]

$$\Phi(\rho) = -\text{Tr}(\rho \ln \rho) - \int_{-\infty}^{0} dt_1 \sum_m G_m(t_1)\text{Tr}(\rho P_m(t_1)) + \lambda \text{Tr}\rho, \tag{5.18}$$

where $G_m(t_1)$ and λ are Lagrange multipliers. From the extremum condition it follows that

$$\delta\Phi(\rho) = -\text{Tr}(\delta\rho \ln \rho) - \text{Tr}(\delta\rho) + \lambda \text{Tr}(\delta\rho) - \int_{-\infty}^{0} dt_1 \sum_m G_m(t_1)\text{Tr}(\delta\rho P_m(t_1)) = 0, \tag{5.19}$$

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hence

$$\rho = \exp\Big(\Lambda - \int_{-\infty}^{0} dt_1 \sum_m G_m(t_1) P_m(t_1)\Big); \quad \Lambda = 1 - \lambda. \tag{5.20}$$

Lagrange multipliers are determined by the conditions (5.17). We have

$$\frac{\delta \tilde{\lambda}}{\delta G_m(t_1)} = \langle P_m(t_1)\rangle^t = -\langle P_m\rangle^{t+t_1}. \tag{5.21}$$

If P_m are integrals of motion, then the statistical operator ρ (5.20) should give the Gibbs distribution, i.e. integral $\int_{-\infty}^{0} dt_1 \sum_m G_m(t_1)$ should be convergent to a constant. It can be obtained if we put $G_m(t_1) = \varepsilon e^{\varepsilon t_1} F_m$. Taking into account this property and the relation (5.14) we get that it is convenient to choose Lagrange multipliers in the form [5]

$$G_m(t_1) = \varepsilon e^{\varepsilon t_1} F_m(t + t_1). \tag{5.22}$$

Then we shall obtain the statistical operator in the form (5.20), which corresponds to the extremum of the information entropy for a given average $\langle P_m\rangle^{t_1}$ in an arbitrary moment of the past. The above consideration shows that the nonequilibrium statistical operator ρ can be written as

$$\rho = \exp(\overline{\ln \rho_q}) = \exp\Big(\varepsilon \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \exp\Big(\frac{iHt_1}{\hbar}\Big) \ln \rho_q(t + t_1) \exp\Big(\frac{-iHt_1}{\hbar}\Big)\Big) = \tag{5.23}$$

$$\exp\Big(-\overline{S(t,0)}\Big) = \exp\Big(-\varepsilon \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} S(t + t_1, t_1)\Big)$$

$$= \exp\Big(-S(t,0) + \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \dot{S}(t + t_1, t_1)\Big).$$

Here

$$\dot{S}(t,0) = \frac{\partial S(t,0)}{\partial t} + \frac{1}{i\hbar}[S(t,0), H]; \quad \dot{S}(t,t_1) = \exp\Big(\frac{iHt_1}{\hbar}\Big) \dot{S}(t,0) \exp\Big(\frac{-iHt_1}{\hbar}\Big). \tag{5.24}$$

It is required [5] that the normalization of statistical operator ρ_q is preserved as well as the statistical operator ρ, and the constraint $\langle P_m\rangle^t = \langle P_m\rangle_q^t$ is fulfilled. For the particular choice of F_m which corresponds to the statistical equilibrium we obtain $\rho = \rho_q = \rho_0$ and $\Lambda = \lambda$. It determines the parameters $F_m(t)$ such that P_m and $F_m(t)$ are thermodynamically conjugate, i.e.

$$\frac{\delta \lambda}{\delta F_m} = -\langle P_m\rangle_q = -\langle P_m\rangle. \tag{5.25}$$

It should be noted that a close related consideration can also be carried out with a deeper concept, the methods of quasiaverages [5, 62, 63]. Zubarev showed [63] that the concepts of symmetry breaking perturbations and quasiaverages [62, 64] play important role in the theory of irreversible processes as well. The method of the construction of the nonequilibrium statistical operator becomes especially deep and transparent when it is applied in the framework of the quasiaverage concept. The main idea of this approach was to consider infinitesimally small sources breaking the time-reversal symmetry of the Liouville equation, which become vanishingly small after a thermodynamic limiting transition.

Let us emphasize once again that the quantum Liouville equation, like the classical one, is symmetric under time-reversal transformation. However, the solution of the Liouville equation is unstable with respect to small perturbations violating this symmetry of the equation. Indeed, let us consider the Liouville equation with an infinitesimally small source into the right-hand side

$$\frac{\partial \rho_\varepsilon}{\partial t} + \frac{1}{i\hbar}[\rho_\varepsilon, H] = -\varepsilon(\rho_\varepsilon - \rho_q), \tag{5.26}$$

or equivalently

$$\frac{\partial \ln \rho_\varepsilon}{\partial t} + \frac{1}{i\hbar}[\ln \rho_\varepsilon, H] = -\varepsilon(\ln \rho_\varepsilon - \ln \rho_q), \tag{5.27}$$

where $(\varepsilon \to 0)$ after the thermodynamic limit. The equation (5.26) is analogous to the corresponding equation of the quantum scattering theory [5, 63]. The introduction of infinitesimally small sources into the Liouville equation is equivalent to the boundary condition

$$\exp\left(\frac{iHt_1}{\hbar}\right)(\rho(t+t_1) - \rho_q(t+t_1))\exp\left(\frac{-iHt_1}{\hbar}\right) \to 0, \tag{5.28}$$

where $t_1 \to -\infty$ *after* the thermodynamic limiting process. It was shown [5, 63] that we can rewrite the nonequilibrium statistical operator in the following useful form:

$$\rho(t,0) = \exp\left(-\varepsilon \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \ln \rho_q(t+t_1, t_1)\right) = \exp\overline{(\ln \rho_q(t,0))} \equiv \exp\overline{(-S(t,0))}. \tag{5.29}$$

The average value of any dynamic variable A is given by

$$\langle A \rangle = \lim_{\varepsilon \to 0^+} \mathrm{Tr}(\rho(t,0)A), \tag{5.30}$$

and is, in fact, the quasiaverage. The normalization of the quasi-equilibrium distribution ρ_q will persists after taking the invariant part if the following conditions will be fulfilled

$$\mathrm{Tr}(\rho(t,0)P_m) = \langle P_m \rangle = \langle P_m \rangle_q; \quad \mathrm{Tr}\rho = 1. \tag{5.31}$$

A short remark about the maximum entropy principle [5, 15, 25, 26, 27, 54] will not be out of the place here. The approach to the nonequilibrium statistical mechanics which is based on the nonequilibrium ensembles is related deeply with that principle, which was used in the NSO method as one of the foundational issue. There are a few slightly different equivalent possibilities of using the maximum entropy principle in this context, which were discussed thoroughly in Refs. [65, 66].

6   Generalized Kinetic Equations

It is well known that kinetic equations are of great interest in the theory of transport processes [1, 2, 5, 15, 16, 67]. The dynamic behavior of charge, magnetic, and lattice systems is of interest for the study of transport processes in solids [15, 16, 17, 18, 67]. The degrees of freedom in solids can often be represented as a few interacting subsystems (electrons, spins, phonons, nuclear spins, etc.). Perturbation of one subsystem may produce a nonequilibrium state which is then relaxed to an equilibrium state due to the interaction between particles or with a thermal bath.

The method of the nonequilibrium statistical operator is a very useful tool to analyze and derive generalized transport and kinetic equations [5, 16, 17, 18, 68]. The generalized kinetic equations were derived by this method by Pokrovski [5, 68] for the case of many-particle system with small interactions among particles. Indeed, as it was shown in the preceding section, the main quantities involved are the following thermodynamically conjugate values:

$$\langle P_m \rangle = -\frac{\delta \Omega}{\delta F_m(t)}; \quad F_m(t) = \frac{\delta S}{\delta \langle P_m \rangle}. \tag{6.1}$$

The generalized transport equations which describe the *time evolution* of variables $\langle P_m \rangle$ and F_m follow from the equation of motion for the P_m, averaged with the nonequilibrium statistical operator (5.29). These equations have the form

$$\langle \dot{P}_m \rangle = -\sum_n \frac{\delta^2 \Omega}{\delta F_m(t) \delta F_n(t)} \dot{F}_n(t); \quad \dot{F}_m(t) = \sum_n \frac{\delta^2 S}{\delta \langle P_m \rangle \delta \langle P_n \rangle} \langle \dot{P}_n \rangle. \tag{6.2}$$

The entropy production has the form

$$\dot{S}(t) = \langle \dot{S}(t,0) \rangle = -\sum_m \langle \dot{P}_m \rangle F_m(t) = -\sum_{n,m} \frac{\delta^2 \Omega}{\delta F_m(t) \delta F_n(t)} \dot{F}_n(t) F_m(t). \tag{6.3}$$

These equations are the mutually conjugate and with Eq.(5.29) form a complete system of equations for the calculation of values $\langle P_m \rangle$ and F_m.

Within the NSO method the derivation of the kinetic equations for a system of weakly interacting particles was carried out by Pokrovski [68]. In this case the Hamiltonian can be written in the form

$$H = H_0 + V, \tag{6.4}$$

where H_0 is the Hamiltonian of noninteracting particles (or quasiparticles) and V is the operator describing the weak interaction among them. Let us choose the set of operators $P_m = P_k$ whose average values correspond to the particle distribution functions, e.g., $a_k^\dagger a_k$ or $a_k^\dagger a_{k+q}$. Here $a_k^\dagger$ and a_k are the creation and annihilation second quantized operators (Bose or Fermi type). These operators obey the following quantum equation of motion: $\dot{P}_k = 1/i\hbar [P_k, H]$. The averaging of this equation with NSO gives the generalized kinetic equations for $\langle P_k \rangle$

$$\frac{d\langle P_k \rangle}{dt} = \frac{1}{i\hbar} \langle [P_k, H] \rangle = \frac{1}{i\hbar} \sum_l c_{kl} \langle P_l \rangle + \frac{1}{i\hbar} \langle [P_k, V] \rangle. \tag{6.5}$$

Hence the calculation of the r.h.s. of (6.5) leads to the explicit expressions for the "collision integral" (collision terms). Since the interaction is small, it is possible to rewrite Eq.(6.5) in the following form:

$$\frac{d\langle P_k \rangle}{dt} = L_k^0 + L_k^1 + L_k^{21} + L_k^{22}, \tag{6.6}$$

where

$$L_k^0 = \frac{1}{i\hbar} \sum_l c_{kl} \langle P_l \rangle_q; \qquad L_k^1 = \frac{1}{i\hbar} \langle [P_k, V] \rangle_q, \tag{6.7}$$

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$$L_k^{21} = \frac{1}{\hbar^2} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle [V(t_1), [P_k, V]] \rangle_q, \tag{6.8}$$

$$L_k^{22} = \frac{1}{\hbar^2} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle [V(t_1), i\hbar \sum_l P_l \frac{\partial L_k^1(\ldots \langle P_l \rangle \ldots)}{\partial \langle P_l \rangle}] \rangle_q. \tag{6.9}$$

The higher order terms proportional to the V^3, V^4, etc., can be derived straightforwardly.

7 System in Thermal Bath

In papers [16, 17, 67, 69] the generalized kinetic equations for the system weakly coupled to a thermal bath have been derived. Examples of such system can be an atomic (or molecular) system interacting with the electromagnetic field it generates as with a thermal bath, a system of nuclear or electronic spins interacting with the lattice, etc. The aim was to describe the relaxation processes in two weakly interacting subsystems, one of which is in the nonequilibrium state and the other is considered as a thermal bath. The concept of thermal bath or heat reservoir, i.e., a system that has effectively an infinite number of degrees of freedom, was not formulated precisely. A standard definition of the thermal bath is a heat reservoir defining a temperature of the system environment. From a mathematical point of view [3, 70], a heat bath is something that gives a stochastic influence on the system under consideration. The problem of a small system weakly interacting with a heat reservoir has various aspects. Basic to the derivation of a transport equation for a small system weakly interacting with a heat bath is a proper introduction of model assumptions. We are interested here in the problem of derivation of the kinetic equations for a certain set of average values (occupation numbers, spins, etc.) which characterize the nonequilibrium state of the system.

The Hamiltonian of the total system was taken in the following form:

$$H = H_1 + H_2 + V, \tag{7.1}$$

where

$$H_1 = \sum_\alpha E_\alpha a_\alpha^\dagger a_\alpha; \quad V = \sum_{\alpha,\beta} \Phi_{\alpha\beta} a_\alpha^\dagger a_\beta, \quad \Phi_{\alpha\beta} = \Phi_{\beta\alpha}^\dagger. \tag{7.2}$$

Here H_1 is the Hamiltonian of the small subsystem, and $a_\alpha^\dagger$ and a_α are the creation and annihilation second quantized operators of quasiparticles in the small subsystem with energies E_α, V is the operator of the interaction between the small subsystem and the thermal bath, and H_2 is the Hamiltonian of the thermal bath which we do not write explicitly. The quantities $\Phi_{\alpha\beta}$ are the operators acting on the thermal bath variables.

We assume that the state of this system is determined completely by the set of averages $\langle P_{\alpha\beta} \rangle = \langle a_\alpha^\dagger a_\beta \rangle$ and the state of the thermal bath by $\langle H_2 \rangle$, where $\langle \ldots \rangle$ denotes the statistical average with the nonequilibrium statistical operator, which will be defined below. We take the quasi-equilibrium statistical operator ρ_q in the form

$$\rho_q(t) = \exp(-S(t,0)), \quad S(t,0) = \Omega(t) + \sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t) + \beta H_2. \tag{7.3}$$

Here $F_{\alpha\beta}(t)$ are the thermodynamic parameters conjugated with $P_{\alpha\beta}$, and β is the reciprocal temperature of the thermal bath; $\Omega = \ln \operatorname{Tr} \exp(-\sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t) - \beta H_2)$. The nonequilibrium statistical operator has the form

$$\rho(t) = \exp(-\overline{S(t,0)}); \quad \overline{S(t,0)} = \varepsilon \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \left(\Omega(t + t_1) + \sum_{\alpha\beta} P_{\alpha\beta} F_{\alpha\beta}(t) + \beta H_2 \right). \quad (7.4)$$

The parameters $F_{\alpha\beta}(t)$ are determined from the condition $\langle P_{\alpha\beta} \rangle = \langle P_{\alpha\beta} \rangle_q$.

In the derivation of the kinetic equations we use the perturbation theory in a *weakness of interaction* and assume that the equality $\langle \Phi_{\alpha\beta} \rangle_q = 0$ holds, while other terms can be added to the renormalized energy of the subsystem. We now turn to the derivation of the kinetic equations. The starting point is the kinetic equations in the following implicit form:

$$\frac{d\langle P_{\alpha\beta} \rangle}{dt} = \frac{1}{i\hbar} \langle [P_{\alpha\beta}, H] \rangle = \frac{1}{i\hbar} (E_\beta - E_\alpha) \langle P_{\alpha\beta} \rangle + \frac{1}{i\hbar} \langle [P_{\alpha\beta}, V] \rangle. \quad (7.5)$$

We restrict ourselves to the second-order in powers of V in calculating the r.h.s. of (7.5). Finally we obtain the kinetic equations for $\langle P_{\alpha\beta} \rangle$ in the form [17, 67, 69]

$$\frac{d\langle P_{\alpha\beta} \rangle}{dt} = \frac{1}{i\hbar} (E_\beta - E_\alpha) \langle P_{\alpha\beta} \rangle - \frac{1}{\hbar^2} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle [[P_{\alpha\beta}, V], V(t_1)] \rangle_q. \quad (7.6)$$

The last term of the right-hand side of Eq.(7.6) can be called the generalized *collision integral*. Thus, we can see that the collision term for the system weakly coupled to the thermal bath has a convenient form of the double commutator as for the generalized kinetic equations [68] for the system with small interaction. It should be emphasized that the assumption about the model form of the Hamiltonian (7.1) is nonessential for the above derivation [16, 17, 67, 69]. The equation (7.6) will be fulfilled for general form of the Hamiltonian of a small system weakly coupled to a thermal bath.

Having shown the derivation of the generalized kinetic equations, we note in this context that investigation of quantum dynamics in the condensed phase is one of a major objective of many recent studies [15, 16, 71]. One of the useful approaches to quantum dynamics in the condensed phase is based on a reduced density matrix approach. An equation of motion for the reduced density matrix was obtained by averaging out of the full density matrix irrelevant bath degrees of freedom which indirectly appear in observations via coupling to the system variables. A well known standard reduced density matrix approach is the Redfield's equations, which were derived also within the NSO formalism [15, 16, 71]. We derived above the kinetic equations for $\langle P_{\alpha\beta} \rangle$ in general form. It is possible to rewrite the kinetic equations for $\langle P_{\alpha\beta} \rangle$ as

$$\frac{d\langle P_{\alpha\beta} \rangle}{dt} = \frac{1}{i\hbar} (E_\beta - E_\alpha) \langle P_{\alpha\beta} \rangle -$$
$$\sum_{\nu} \left(K_{\beta\nu} \langle P_{\alpha\nu} \rangle + K_{\alpha\nu}^{\dagger} \langle P_{\nu\beta} \rangle \right) + \sum_{\mu\nu} K_{\alpha\beta,\mu\nu} \langle P_{\mu\nu} \rangle. \quad (7.7)$$

For notation see Refs. [15, 16] The above result is similar in structure to the Redfield's equation for the spin density matrix [15] when the external time-dependent field is absent.

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Indeed, the Redfield's equation of motion for the spin density matrix has the form [15]

$$\frac{\partial \rho^{\alpha\alpha'}}{\partial t} = -i\omega_{\alpha\alpha'}\rho^{\alpha\alpha'} + \sum_{\beta\beta'} R_{\alpha\alpha'\beta\beta'}\rho^{\beta\beta'}.$$

Here $\rho^{\alpha\alpha'}$ is the α, α' matrix element of the spin density matrix, $\omega_{\alpha\alpha'} = (E_\alpha - E_{\alpha'})\hbar$, where E_α is energy of the spin state α and $R_{\alpha\alpha'\beta\beta'}\rho^{\beta\beta'}$ is the "relaxation matrix". A sophisticated analysis and derivation of the Redfield's equation for the density of a spin system immersed in a thermal bath was given in [15, 16].

Returning to Eq.(7.7), it is it can be shown, that if one confines himself to the diagonal averages $\langle P_{\alpha\alpha} \rangle$ only, this equation may be transformed to give [15, 16, 67, 69]

$$\frac{d\langle P_{\alpha\alpha} \rangle}{dt} = \sum_\nu K_{\alpha\alpha,\nu\nu}\langle P_{\nu\nu} \rangle - \left(K_{\alpha\alpha} + K_{\alpha\alpha}^\dagger \right)\langle P_{\alpha\alpha} \rangle, \tag{7.8}$$

$$K_{\alpha\alpha,\beta\beta} = \frac{1}{\hbar^2} J_{\alpha\beta,\beta\alpha}\left(\frac{E_\alpha - E_\beta}{\hbar}\right) = W_{\beta\to\alpha}, \tag{7.9}$$

$$K_{\alpha\alpha} + K_{\alpha\alpha}^\dagger = \frac{1}{\hbar^2} \sum_\beta J_{\beta\alpha,\alpha\beta}\left(\frac{E_\beta - E_\alpha}{\hbar}\right) = W_{\alpha\to\beta}. \tag{7.10}$$

Here $W_{\beta\to\alpha}$ and $W_{\alpha\to\beta}$ are the transition probabilities expressed in the spectral intensity terms. Using the properties of the spectral intensities [5], it is possible to verify that the transition probabilities satisfy the relation of the detailed balance

$$\frac{W_{\beta\to\alpha}}{W_{\alpha\to\beta}} = \frac{\exp(-\beta E_\alpha)}{\exp(-\beta E_\beta)}. \tag{7.11}$$

Finally, we have

$$\frac{d\langle P_{\alpha\alpha} \rangle}{dt} = \sum_\nu W_{\nu\to\alpha}\langle P_{\nu\nu} \rangle - \sum_\nu W_{\alpha\to\nu}\langle P_{\alpha\alpha} \rangle. \tag{7.12}$$

This equation has the usual form of the Pauli master equation. It is known that the master equation is an ordinary differential equation describing the *reduced evolution* of the system obtained from the full Heisenberg evolution by taking the partial expectation with respect to the vacuum state of the reservoirs degrees of freedom. In this sense, the generalized master equation is a tool for extracting the dynamics of a subsystem of a larger system by the use of a special projection techniques [11], or special expansion technique [15, 16].

8   Schrödinger-Type Equation with Damping

The problem of the inclusion of dissipative forces in quantum mechanics is of great interest. There are various approaches to this complicated problem [15, 16]. The inclusion of dissipative forces in quantum mechanics through the use of non-Hermitian Hamiltonians is of great interest in the theory of interaction between heavy ions. It is clear that if the Hamiltonian has a non-Hermitian part H_A, the Heisenberg equation of motion will be modified

by additional terms. However, care must be taken in defining the probability density operator when the Hamiltonian is non-Hermitian. The necessity of considering such processes arises in the description of various quantum phenomena (e.g. radiation damping, etc.), since quantum systems experience dissipation and fluctuations through interaction with a reservoir [15, 16, 67]. Here we consider the behavior of a small dynamic system interacting with a thermal bath, i.e., with a system that has effectively an infinite number of degrees of freedom, in the approach of the nonequilibrium statistical operator [15, 16, 72], on the basis of the equations described in previous section. It was assumed that the dynamic system (system of particles) is far from equilibrium with the thermal bath and cannot, in general, be characterized by a temperature. As a result of interaction with the thermal bath, such a system acquires some statistical characteristics but remains essentially a mechanical system. Our aim was to obtain an equation of evolution (equations of motion) for the relevant variables which are characteristic of the system under consideration [15, 16, 72]. The basic idea was to eliminate effectively the thermal bath variables. The influence of the thermal bath will be manifested then as an *effect of friction* of the particle in a medium. The presence of friction leads to dissipation and, thus, to irreversible processes. In other words, it was supposed that the reservoir can be *completely eliminated*, provided that the frequency shifts and dissipation induced by the reservoir are incorporated into the properly averaged equations of motion, and provided that a suitable operator *noise source* with the correct moments are added.

Let us consider the behavior of a small subsystem with Hamiltonian H_1 interacting with a thermal bath with Hamiltonian H_2. The total Hamiltonian has the form (7.1). As operators P_m determining the nonequilibrium state of the small subsystem, we take $a_\alpha^\dagger, a_\alpha$, and $n_\alpha = a_\alpha^\dagger a_\alpha$. Note that the choice of only the operators n_α and H_2 would lead to kinetic equations (7.6) for the system in the thermal bath derived above.

The quasi-equilibrium statistical operator (7.3) is determined from the extremum of the information entropy, subjected to the additional conditions that the quantities

$$\mathrm{Tr}(\rho a_\alpha) = \langle a_\alpha \rangle, \quad \mathrm{Tr}(\rho a_\alpha^\dagger) = \langle a_\alpha^\dagger \rangle, \quad \mathrm{Tr}(\rho n_\alpha) = \langle n_\alpha \rangle \qquad (8.1)$$

remain constant during the variation and the normalization $\mathrm{Tr}(\rho) = 1$ is preserved. The operator ρ_q has the form

$$\rho_q = \exp\left(\Omega - \sum_\alpha (f_\alpha(t)a_\alpha + f_\alpha^\dagger(t)a_\alpha^\dagger + F_\alpha(t)n_\alpha) - \beta H_2\right) \equiv \exp(-S(t,0)). \qquad (8.2)$$

Here, $f_\alpha, f_\alpha^\dagger$ and F_α are Lagrangian multipliers determined by the conditions (8.1). They are the parameters conjugate to $\langle a_\alpha \rangle_q, \langle a_\alpha^\dagger \rangle_q$ and $\langle n_\alpha \rangle_q$:

$$\langle a_\alpha \rangle_q = -\frac{\delta \Omega}{\delta f_\alpha(t)}, \quad \langle n_\alpha \rangle_q = -\frac{\delta \Omega}{\delta F_\alpha(t)}, \quad \frac{\delta S}{\delta \langle a_\alpha \rangle_q} = f_\alpha(t), \quad \frac{\delta S}{\delta \langle n_\alpha \rangle_q} = F_\alpha(t). \qquad (8.3)$$

It is worth noting that our choice of the relevant operators $\langle a_\alpha \rangle_q, \langle a_\alpha^\dagger \rangle_q$ precisely corresponds to the ideas of the McLennan, described above. His method is based on the introduction of external forces of a nonconservative nature, which describe the influence of the surroundings or of a thermal bath on the given system. Indeed, our choice means introduction of artificial external forces, which broke the law of the particle conservation. This is especially radical

view for the case of Fermi-particles, since it broke the spin conservation law too [73].
In what follows, it is convenient to write the quasi-equilibrium statistical operator (7.3) in the factorized form $\rho_q = \rho_1 \bigotimes \rho_2$. Here the notation are:

$$\rho_1 = \exp\left(\Omega_1 - \sum_\alpha (f_\alpha(t)a_\alpha + f_\alpha^\dagger(t)a_\alpha^\dagger + F_\alpha(t)n_\alpha)\right), \quad \rho_2 = \exp\left(\Omega_2 - \beta H_2\right). \qquad (8.4)$$

The nonequilibrium statistical operator ρ will have the form (7.4). Note, that the following conditions are satisfied:

$$\langle a_\alpha \rangle_q = \langle a_\alpha \rangle, \quad \langle a_\alpha^\dagger \rangle_q = \langle a_\alpha^\dagger \rangle, \quad \langle n_\alpha \rangle_q = \langle n_\alpha \rangle. \qquad (8.5)$$

We shall take, as our starting point, the equations of motion for the operators averaged with the nonequilibrium statistical operator

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = \langle [a_\alpha, H_1] \rangle + \langle [a_\alpha, V] \rangle, \quad i\hbar \frac{d\langle n_\alpha \rangle}{dt} = \langle [n_\alpha, H_1] \rangle + \langle [n_\alpha, V] \rangle. \qquad (8.6)$$

The equation for $\langle a_\alpha^\dagger \rangle$ can be obtained by taking the conjugate of (8.6). Restricting ourselves to the second order in the interaction V, we obtain, by analogy with (7.6), the following equations [15, 16, 72]:

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \frac{1}{i\hbar} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle [[a_\alpha, V], V(t_1)] \rangle_q, \qquad (8.7)$$

$$i\hbar \frac{d\langle n_\alpha \rangle}{dt} = \frac{1}{i\hbar} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle [[n_\alpha, V], V(t_1)] \rangle_q. \qquad (8.8)$$

Here $V(t_1)$ denotes the interaction representation of the operator V. Expanding the double commutator in Eq.(8.7), we obtain

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle$$

$$+ \frac{1}{i\hbar} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \left(\sum_{\beta\mu\nu} \langle \Phi_{\alpha\beta} \phi_{\mu\nu}(t_1) \rangle_q \langle a_\beta a_\mu^\dagger a_\nu \rangle_q - \langle \phi_{\mu\nu}(t_1) \Phi_{\alpha\beta} \rangle_q \langle a_\mu^\dagger a_\nu a_\beta \rangle_q \right), \qquad (8.9)$$

where $\phi_{\mu\nu}(t_1) = \Phi_{\mu\nu}(t_1) \exp\left(i/\hbar(E_\mu - E_\nu)t_1\right)$. We assume that the terms of higher order than linear can be dropped. Then we get

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \frac{1}{i\hbar} \sum_{\beta\mu} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle \Phi_{\alpha\mu} \phi_{\mu\beta}(t_1) \rangle_q \langle a_\beta \rangle. \qquad (8.10)$$

The form of the linear equation (8.10) is the same for Bose and Fermi statistics.
Using the spectral representations [5, 72], it is possible to rewrite Eq.(8.10) by analogy with Eq.(7.8) as

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \sum_\beta K_{\alpha\beta} \langle a_\beta \rangle. \qquad (8.11)$$

Thus, we have obtained the equation of motion for the average $\langle a_\alpha \rangle$. It is clear that this equation describes approximately the evolution of the state of the dynamic system interacting with the thermal bath. The last term in the right-hand side of this equation leads to the shift of energy E_α and to the damping due to the interaction with the thermal bath (or medium). In a certain sense, it is possible to say that Eq.(8.11) is an analog or the generalization of the Schrödinger equation [15, 16, 72].

It is of interest to analyze and track more closely the analogy with the Schrödinger equation in the coordinate form. To do this, by convention, we define the "*wave function*"

$$\psi(\mathbf{r}) = \sum_\alpha \chi_\alpha(\mathbf{r})\langle a_\alpha \rangle, \tag{8.12}$$

where $\{\chi_\alpha(\mathbf{r})\}$ is a complete orthonormalized system of single-particle functions of the operator $(-\hbar^2/2m\nabla^2 + v(\mathbf{r}))$, where $v(\mathbf{r})$ is the potential energy, and

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) \right) \chi_\alpha(\mathbf{r}) = E_\alpha \chi_\alpha(\mathbf{r}). \tag{8.13}$$

Thus, in a certain sense, the quantity $\psi(\mathbf{r})$ may plays the role of the wave function of a particle in a medium. Now, using (8.12), we transform Eq.(8.11) to (see Refs. [16, 17, 67, 72])

$$i\hbar\frac{\partial \psi(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) \right) \psi(\mathbf{r}) + \int K(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}'. \tag{8.14}$$

The kernel $K(\mathbf{r}, \mathbf{r}')$ of the integral equation (8.14) has the form

$$K(\mathbf{r}, \mathbf{r}') = \sum_{\alpha\beta} K_{\alpha\beta}\chi_\alpha(\mathbf{r})\chi_\beta^\dagger(\mathbf{r}') = \frac{1}{i\hbar}\sum_{\alpha,\beta,\mu}\int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle \Phi_{\alpha\mu}\phi_{\mu\beta}(t_1)\rangle_q \chi_\alpha(\mathbf{r})\chi_\beta^\dagger(\mathbf{r}'). \tag{8.15}$$

Equation (8.14) can be called a *Schrödinger-type equation* with damping for a dynamical system in a thermal bath. It is interesting to note that similar Schrödinger equations with a nonlocal interaction are used in the scattering theory [15] to describe interaction with many scattering centers.

To demonstrate the capabilities of equation (8.14), it is convenient to introduce the operator of translation $\exp(i\mathbf{q}\mathbf{p}/\hbar)$, where $\mathbf{q} = \mathbf{r}' - \mathbf{r}$; $\mathbf{p} = -i\hbar\nabla_r$. Then Eq.(8.14) can be rewritten in the form

$$i\hbar\frac{\partial \psi(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) \right) \psi(\mathbf{r}) + \sum_p D(\mathbf{r}, \mathbf{p})\psi(\mathbf{r}), \tag{8.16}$$

where

$$D(\mathbf{r}, \mathbf{p}) = \int d^3q K(\mathbf{r}, \mathbf{r} + \mathbf{q}) \exp\left(\frac{i\mathbf{q}\mathbf{p}}{\hbar}\right). \tag{8.17}$$

It is reasonable to assume that the wave function $\psi(\mathbf{r})$ varies little over the correlation length characteristic of the kernel $K(\mathbf{r}, \mathbf{r}')$. Then, expanding $\exp(i\mathbf{q}\mathbf{p}/\hbar)$ in a series, we obtain the following equation in the zeroth order:

$$i\hbar\frac{\partial \psi(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) + \mathrm{Re}U(\mathbf{r}) \right) \psi(\mathbf{r}) + i\,\mathrm{Im}U(\mathbf{r})\psi(\mathbf{r}), \tag{8.18}$$

where

$$U(\mathbf{r}) = \operatorname{Re}U(\mathbf{r}) + i\operatorname{Im}U(\mathbf{r}) = \int d^3q K(\mathbf{r}, \mathbf{r} + \mathbf{q}). \tag{8.19}$$

Expression (8.18) has the form of a Schrödinger equation with a complex potential. Equations of this form are well known in the scattering theory [15], in which one introduces an interaction describing absorption ($\operatorname{Im}U(\mathbf{r}) < 0$). Let us consider the expansion of $\exp\left(i\mathbf{q}\mathbf{p}/\hbar\right)$ in Eq.(8.17) in a series up to second order inclusively. Then we can represent Eq.(8.14) in the form [16, 67, 72]

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t} = \left\{ \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) \right) + U(\mathbf{r}) - \frac{1}{i\hbar}\int d\mathbf{r}' K(\mathbf{r}, \mathbf{r} + \mathbf{r}')\mathbf{r}'\mathbf{p} \right. \tag{8.20}$$

$$\left. + \frac{1}{2}\int K(\mathbf{r}, \mathbf{r} + \mathbf{r}')d\mathbf{r}' \sum_{i,k=1}^{3} r_i' r_k' \nabla_i \nabla_k \right\} \psi(\mathbf{r}).$$

Let us introduce the function

$$\mathbf{A}(\mathbf{r}) = \frac{mc}{i\hbar e}\int d\mathbf{r}' K(\mathbf{r}, \mathbf{r} + \mathbf{r}')\mathbf{r}', \tag{8.21}$$

which, in a certain sense, is the analog of the complex vector potential of an electromagnetic field. Then we can define an analog of the tensor of the reciprocal effective masses, considered in details in Refs. [15, 67, 74]

$$\left\{ \frac{1}{M(\mathbf{r})} \right\}_{ik} = \frac{1}{m}\delta_{ik} - \int d\mathbf{r}' \operatorname{Re}K(\mathbf{r}, \mathbf{r} + \mathbf{r}')r_i' r_k'. \tag{8.22}$$

Hence we can rewrite Eq.(8.14) in the form

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t} \tag{8.23}$$

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

where

$$T(\mathbf{r}) = \frac{1}{2}\int d\mathbf{r}' \operatorname{Im}K(\mathbf{r}, \mathbf{r} + \mathbf{r}')\sum_{i,k} r_i' r_k' \nabla_i \nabla_k. \tag{8.24}$$

In the case of an isotropic medium, the tensor $\left\{ 1/M(\mathbf{r}) \right\}_{ik}$ is diagonal and $\mathbf{A}(\mathbf{r}) = 0$.

It is worth while to mention that the transmission and scattering problems involving complex potentials are important in physics, in particular in describing nuclear collisions [15]. Note, that the introduction of $\psi(\mathbf{r})$ does not mean that the state of the small dynamical subsystem is pure. It remains mixed since it is described by the statistical operator (8.4), the evolution of the parameters f_α, $f_\alpha^\dagger$, and F_α of the latter being governed by a coupled system of equations of Schrödinger and kinetic types.

Hence, we have shown in this section that for some class of dynamic systems it was possible, with the NSO approach, to go from a Hamiltonian description of dynamics to a description in terms of processes which incorporates the dissipation [15, 16, 17, 67, 72]. However, a careful examination is required in order to see under what conditions the Schrödinger-type equation with damping can really be used.

9 Damping Effects in Open Dynamical System

In order to clarified this point and to interpret properly the physical meaning of the derived equations, the example will be considered here. Let us consider briefly important example [75] of the application of the Schrödinger-type equation with damping. We consider the problem of the natural width of spectral line of the atomic system and show that our result coincides with the results obtained earlier by other methods. It is well known that the excited levels of the isolated atomic system have a finite lifetime because there is a probability of emission of photons due to interaction with the self-electromagnetic field. This leads to the atomic levels becoming quasi-discrete and consequently acquiring a finite small width. It is just this width that is called the *natural width* of the spectral lines.

Let us consider an atom interacting with the self-electromagnetic field in the approximation when the atom is at rest. For simplicity, the atom is supposed to be in two states only, i.e. in a ground state a and in an excited state b. The atomic system in the excited state b is considered, in a certain sense, as a small "nonequilibrium" system, and the self-electromagnetic field as a "thermostat" or a "thermal bath". The relaxation of the small system is then a decay of the excited level and occurs by radiative transitions.

We shall not discuss here the case when the electromagnetic field can be considered as an equilibrium system with infinitely many degrees of freedom, because it has been discussed completely in the literature. We write the total Hamiltonian in the form $H = H_{at} + H_f + V$, where

$$H_{at} = \sum_\alpha E_\alpha a_\alpha^\dagger a_\alpha \tag{9.1}$$

is the Hamiltonian for the atomic system alone, $a_\alpha^\dagger$ and a_α are the creation and annihilation operators of the system in the state with energy E_α.

$$H_f = \sum_{k,\lambda} kc b_{k,\lambda}^\dagger b_{k,\lambda} \tag{9.2}$$

is the Hamiltonian of transverse electromagnetic field [15, 75], $\lambda = 1, 2$ is the polarization, $\hbar \mathbf{k}$ is the momentum of a photon, $b_{k,\lambda}^\dagger$ and $b_{k,\lambda}$ are the creation and annihilation operators of the photon in the state $(\mathbf{k}\lambda)$, c is the light velocity, V is the interaction operator responsible for the radiative transitions and having the following form in the non-relativistic approximation

$$V = -\frac{e}{mc} \mathbf{p} \cdot \mathbf{A}_{tr}(\mathbf{r}), \tag{9.3}$$

where e and m are the electron charge and mass, respectively, $\mathbf{A}_{tr}(\mathbf{r})$ is the vector-potential of the transverse electromagnetic field at the point $\mathbf{r}$; $[\mathbf{p} \times \mathbf{A}_{tr}(\mathbf{r})] = 0$. For a finite system enclosed in a cubic box of volume Ω with periodic boundary conditions, one can write [15, 75]

$$\mathbf{A}_{tr}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{k,\lambda} \left(\frac{2\pi\hbar^2 c}{k}\right)^{1/2} \mathbf{e}_{k,\lambda} \left(b_{k,\lambda} \exp(\frac{i\mathbf{kr}}{\hbar}) + b_{k,\lambda}^\dagger \exp(-\frac{i\mathbf{kr}}{\hbar})\right). \tag{9.4}$$

Now, following the derivation of section 7, the interaction V is represented as a product, such that the atomic and field variables are factorized:

$$V = \sum_{\alpha,\beta} \varphi_{\alpha\beta} a_\alpha^\dagger a_\beta, \quad \varphi_{\alpha\beta} = \varphi_{\beta\alpha}^\dagger, \tag{9.5}$$

where

$$\varphi_{\alpha\beta} = \frac{1}{\sqrt{\Omega}} \sum_{k,\lambda} \left(G_{\alpha,\beta}(k,\lambda) b_{k,\lambda} + b_{k,\lambda}^{\dagger} G_{\beta\alpha}^{*}(k,\lambda) \right), \tag{9.6}$$

$$G_{\alpha,\beta}(k,\lambda) = -\frac{e}{mc} \left(\frac{2\pi\hbar^2 c}{k} \right)^{1/2} \mathbf{e}_{k,\lambda} \langle \alpha | \exp\left(\frac{i\mathbf{kr}}{\hbar} \right) \cdot \mathbf{p} | \beta \rangle. \tag{9.7}$$

Here $|\alpha\rangle$ and $|\beta\rangle$ are the eigenstates of energies E_α and E_β that of the Hamiltonian H_{at}, and are given by

$$H_{at}|\alpha\rangle = E_\alpha|\alpha\rangle, \quad (\alpha,\beta) = (a,b). \tag{9.8}$$

In the electric-dipole approximation we get

$$\varphi_{\alpha\beta} = -\frac{e}{mc} \langle \alpha | \mathbf{p} | \beta \rangle \sum_{k,\lambda} \left(\frac{2\pi\hbar^2 c}{k} \right)^{1/2} \mathbf{e}_{k,\lambda} (b_{k,\lambda} + b_{k,\lambda}^{\dagger}). \tag{9.9}$$

The matrix element of the dipole moment $\mathbf{d} = e\mathbf{r}$ between states $|\alpha\rangle$ and $|\beta\rangle$ is related to the matrix element of the momentum $\mathbf{p}$ in the following way

$$\langle \alpha | \mathbf{p} | \beta \rangle = -\frac{m}{e\hbar}(E_\alpha - E_\beta)\mathbf{d}_{\alpha\beta}, \tag{9.10}$$

and we assume that $\langle \alpha | \mathbf{p} | \alpha \rangle = 0$.

As was already mentioned, we use the Schrödinger-type equation with damping for the quantity $\langle a_\alpha \rangle$ which has the form

$$i\hbar \frac{d\langle a_\alpha \rangle}{dt} = E_\alpha \langle a_\alpha \rangle + \sum_{\beta} K_{\alpha\beta} \langle a_\beta \rangle, \tag{9.11}$$

where

$$K_{\alpha\beta} = \frac{1}{i\hbar} \sum_{\gamma} \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle \varphi_{\alpha\gamma} \tilde{\varphi}_{\gamma\beta}(t_1) \rangle_q. \tag{9.12}$$

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

$$\tilde{\varphi}_{\alpha\beta}(t) = \varphi_{\alpha\beta}(t) \exp\left[\frac{i}{\hbar}(E_\alpha - E_\beta)t \right]. \tag{9.13}$$

It is clear that the K_{aa} and K_{ba} are equal to zero and thus Eq.(9.11) becomes

$$i\hbar \frac{d\langle a_b \rangle}{dt} = E_b \langle a_b \rangle + K_{bb} \langle a_b \rangle, \tag{9.14}$$

where

$$K_{bb} = \frac{2\pi\hbar^2 e^2}{m^2 c} \frac{1}{\Omega} \sum_{k} \int_{-\infty}^{\infty} d\omega \frac{1}{k} \frac{J(k,\omega)}{\hbar\omega_0 + \hbar\omega + i\varepsilon} A_{ab}^{ab} \left(\frac{\mathbf{k}}{k} \right). \tag{9.15}$$

Here $\hbar\omega_0 = (E_b - E_a)$,

$$J(k,\omega) = ((\langle n_k \rangle + 1)\delta(\omega + ck) + \langle n_k \rangle \delta(\omega - ck)), \tag{9.16}$$

$$\langle n_k \rangle = \sum_{\lambda} \langle n_{k\lambda} \rangle = \left(e^{\beta ck} - 1 \right)^{-1} = n(k), \tag{9.17}$$

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and

$$A_{ab}^{ab} = |\langle a| \, \mathbf{p} \, |b\rangle|^2 - \left(\langle a| \, \mathbf{p} \, |b\rangle \frac{\mathbf{k}}{k} \right) \left(\langle b| \, \mathbf{p} \, |a\rangle \frac{\mathbf{k}}{k} \right). \tag{9.18}$$

Next we have

$$\frac{1}{\Omega} \sum_k \int_{-\infty}^{\infty} d\omega \frac{1}{k} \frac{J(k,\omega)}{\hbar\omega_0 + \hbar\omega + i\varepsilon} A_{ab}^{ab} \left(\frac{\mathbf{k}}{k} \right) = \tag{9.19}$$

$$\frac{1}{(2\pi)^3} \int k \, dk \int_{-\infty}^{\infty} d\omega \frac{1}{k} \frac{J(k,\omega)}{\hbar\omega_0 + \hbar\omega + i\varepsilon} \int A_{ab}^{ab} \left(\frac{\mathbf{k}}{k} \right) d\varpi,$$

where $d\varpi$ denotes the spherical angle element. It can be verified that

$$\int A_{ab}^{ab} \left(\frac{\mathbf{k}}{k} \right) d\varpi = \frac{8\pi}{3} |\langle a| \, \mathbf{p} \, |b\rangle|^2. \tag{9.20}$$

Substitution of Eq.(9.20) into Eq.(9.15) gives ($\nu = ck$, c is the speed of light)

$$K_{bb} = \frac{2e^2}{m^2 c^2 \hbar} |\langle a| \, \mathbf{p} \, |b\rangle|^2 \int_0^{\infty} \nu \, d\nu \left(\frac{n(\nu) + 1}{\omega_0 - \nu + i\varepsilon} + \frac{n(\nu)}{\omega_0 + \nu + i\varepsilon} \right). \tag{9.21}$$

Finally, we obtain the formulae for width Γ_b, which we defined by $K_{bb} = \Delta E_b - (\hbar/2)i\Gamma_b$, from Eq.(9.21) when the temperature tends to zero

$$\Gamma_b = \frac{4}{3} \frac{e^2 \omega_0}{m^2 c^3 \hbar} |\langle a| \, \mathbf{p} \, |b\rangle|^2 = \frac{4}{3} \frac{\omega_0^3}{c^3 \hbar} |\mathbf{d}_{ab}|^2. \tag{9.22}$$

This expression coincides with the well-known value for the natural width of spectral lines. We are not concerned with the calculation of the shift and discussion of its linear divergence because this is a usual example of the divergence of the self-energy in field theories.
Thus, with the aid of the Schrödinger-type equation with damping one can simply calculate the energy width and shift. The Eq.(8.14) was used widely in a number of concrete problems of line broadening due to perturbation [15].

10   Generalized Van Hove Formula

Microscopic descriptions of dynamical behavior of condensed matter use the notion of correlations over space and time [5, 15]. Correlations over space and time in the density fluctuations of a fluid are responsible for the scattering of light when light passes through the fluid. The fluctuating properties are conveniently described in terms of time-dependent correlation functions formed from the basic dynamical variables, e.g. the particle number density. The fluctuation-dissipation theorem [5, 15], shows that the susceptibilities can be expressed in terms of the fluctuating properties of the system in equilibrium. In paper [76] the theory of scattering of particles (e.g. neutrons) by statistical medium was recast for the nonequilibrium statistical medium. The correlation scattering function of the relevant variables give rise to a very compact and entirely general expression for the scattering cross section of interest. The formula obtained by Van Hove [15] provides a convenient method of analyzing the properties of slow neutron and light scattering by systems of particles such

as gas, liquid or solid in the equilibrium state. In the paper [76] the theory of scattering of particles by many-body system was reformulated and generalized for the case of nonequilibrium statistical medium. A method of quantum-statistical derivation the space and time Fourier transforms of the Van Hove correlation function was formulated on the basis of the method of NSO. This expression gives a natural extension of the familiar Van Hove formula for scattering of slow neutrons for the case in which the system under consideration is in a nonequilibrium state.

The differential cross section for the scattering of thermal neutrons may be expressed in terms of microscopic two-time correlation functions of dynamical variables for the target system. For equilibrium systems, the van Hove formalism provides a general approach to a compact treatment of scattering of neutrons (or other particles) by arbitrary systems of atoms in equilibrium [15]. The relation between the cross-sections for scattering of slow neutrons by an assembly of nuclei and space-time correlation functions for the motion of the scattering system has been given by Van Hove in terms of the dynamic structure factor. Van Hove showed that the energy and angle differential cross section is proportional to the double Fourier transform of a time-dependent correlation function $G(\mathbf{r}, t)$. By definition, $G(\mathbf{r}, t)$ is the equilibrium ensemble average of a product of two time-dependent density operators and is therefore closely related to the linear response of the system to an externally induced disturbance.

To formulate it a more precisely, the dynamic structure factor is a mathematical function that contains information about inter-particle correlations and their time evolution. Experimentally, it can be accessed most directly by inelastic neutron scattering. The dynamic structure factor is most often denoted $\mathcal{S}(\mathbf{k}, \omega)$, where $\mathbf{k}$ is a wave vector (a wave number for isotropic materials), and ω a frequency (sometimes stated as energy, $\hbar\omega$). It is the spatial and temporal Fourier transform of van Hove's time-dependent pair correlation function $G(\mathbf{r}, t)$, whose Fourier transform with respect to $\mathbf{r}$, $\mathcal{S}(\mathbf{k}, t)$, is called the intermediate scattering function and can be measured by neutron spin echo spectroscopy. In an isotropic sample (with scalar r), $G(r, t)$ is a time dependent radial distribution function. In contrast with the systems in equilibrium state, no such general approach was formulated for the systems in nonequilibrium state.

It is well known that the basic quantity is measured in the scattering experiment is the partial differential cross-section. We will consider a target as a crystal with lattice period a. Transition amplitude is first order in the perturbation and the probability is consequently second order. A perturbative approximation for the transition probability from an initial state to a final state under the action of a weak potential V is written as

$$W_{kk'} = \frac{2\pi}{\hbar} \left| \int d^3 r \psi_{k'}^* V \psi_k \right|^2 D_{k'}(E'), \tag{10.1}$$

where $D_{k'}(E')$ is the density of final scattered states. Definition of the scattering cross-section is

$$d\sigma = \frac{W_{kk'}}{\text{Incident flux}}. \tag{10.2}$$

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

$$D_{k'}(E') = \frac{1}{(2\pi)^3} \frac{d^3 k'}{dE'} = \frac{m^2}{(2\pi)^3 \hbar^3} d\Omega \left(\frac{\hbar k'}{m} \right). \tag{10.3}$$

Thus, the differential scattering cross-section is written as

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi)^2\hbar^4}\frac{k'}{k}\left|\int d^3r e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}}V(\mathbf{k})\right|^2. \tag{10.4}$$

The general formalism described above can be applied to the particular case of neutron inelastic scattering [15, 76]. A typical experimental situation includes a monochromatic beam of neutrons, with energy E and wave vector $\mathbf{k}$, scattered by a sample or target. Scattered neutrons are analyzed as a function of both their final energy $E' = E + \hbar\omega$, and the direction, $\vec{\Omega}$, of their final wave vector, $\mathbf{k}'$. We are interested in the quantity I, which is the number of neutrons scattered per second, between $\mathbf{k}$ and $\mathbf{k} + d\mathbf{k}$

$$I = I_0\frac{ma^3}{\hbar k}dw(\mathbf{k} \to \mathbf{k}')D(\mathbf{k})d\mathbf{k}. \tag{10.5}$$

Here, m is the neutron mass, a^3 is the sample unit volume and $dw(\mathbf{k} \to \mathbf{k}')$ is the transition probability from the initial state $|\mathbf{k}\rangle$ to the final state $|\mathbf{k}'\rangle$, and $D(\mathbf{k})$ is the density of states of momentum $\mathbf{k}$. It is given by

$$D(\mathbf{k})d\mathbf{k} = \frac{a^3}{(2\pi)^3}k^2 d\vec{\Omega}dk. \tag{10.6}$$

It is convenient to take the following representations for the incident and scattered wave functions of a neutron:

$$\psi_k = \sqrt{\frac{m}{k}}\,e^{\frac{i}{\hbar}(\mathbf{kr})}, \quad \psi_{k'} = \frac{1}{(2\pi\hbar)^{3/2}}\,e^{\frac{i}{\hbar}(\mathbf{k'r})}. \tag{10.7}$$

For the transition amplitude we obtain

$$dw(\mathbf{k} \to \mathbf{k}') = \frac{m}{\hbar^2 k}\frac{dk'_x dk'_y dk'_z}{(2\pi\hbar)^3}\int_\infty^\infty \langle V(\mathbf{r})V(\mathbf{r}',t)\rangle e^{[-i/\hbar(\mathbf{k}-\mathbf{k}')(\mathbf{r}-\mathbf{r}')-i\omega t]}dt d\mathbf{r}d\mathbf{r}'. \tag{10.8}$$

In other words, the transition amplitude which describes the change of the state of the probe per unit time is

$$dw(\mathbf{k} \to \mathbf{k}') = \frac{1}{\hbar^2}\int_\infty^\infty dt \mathrm{Tr}\Big(\rho_m V_{\mathbf{k'k}}(0)V_{\mathbf{k'k}}(t)\Big)\exp(-i\omega t), \tag{10.9}$$

where ρ_m is a statistical matrix of the target.
Thus the partial differential cross-section is written in the form

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{d\vec{\Omega}d\omega}\cdot\frac{I}{I_0}. \tag{10.10}$$

It can be rewritten as

$$\frac{d^2\sigma}{d\Omega dE'} = A\int_\infty^\infty \langle V(\mathbf{r})V(\mathbf{r}',t)\rangle e^{[-i/\hbar(\mathbf{k}-\mathbf{k}')(\mathbf{r}-\mathbf{r}')-i\omega t]}dt d\mathbf{r}d\mathbf{r}', \tag{10.11}$$

where

$$A = \frac{m^2}{(2\pi)^3\hbar^5}\frac{k'}{k}, \quad E' = \frac{k'^2}{2m}. \tag{10.12}$$

Thus the differential scattering cross section (in first Born approximation) for a system of interacting particles is written in the form (10.11), where A is a factor depending upon the momenta of the incoming and outgoing particles and upon the scattering potential for particle scattering, which for neutron scattering may be taken as the Fermi pseudopotential

$$V = \frac{2\pi\hbar^2}{m} \sum_i b_i \delta(\mathbf{r} - \mathbf{R}_i). \tag{10.13}$$

Here $\mathbf{R}_i$ is the position operator of nuclei in the target and b_i is the corresponding scattering length. It should be taken into account that

$$V = \sum_{i=1}^{N} V(\mathbf{r} - \mathbf{R}_i) = \sum_{i=1}^{N} e^{-\frac{i}{\hbar}(\mathbf{pR}_i)} V(\mathbf{r}) e^{\frac{i}{\hbar}(\mathbf{pR}_i)}, \tag{10.14}$$

and

$$\langle \beta\, \mathbf{k}' | V | \alpha\, \mathbf{k} \rangle = \langle \mathbf{k}' | V(\mathbf{r}) | \mathbf{k} \rangle \sum_{i=1}^{N} \langle \beta | e^{-\frac{i}{\hbar}(\mathbf{k}'\mathbf{R}_i)} e^{\frac{i}{\hbar}(\mathbf{kR}_i)} | \alpha \rangle. \tag{10.15}$$

Thus we obtain

$$\frac{d^2\sigma}{d\Omega dE'} \propto \frac{k'}{k} \frac{1}{2\pi} \sum_{ij} \int_{-\infty}^{\infty} \frac{1}{N} b_i b_j \left\langle \exp[\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_i(0)] \exp[-\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_j(t)] \right\rangle \exp(-i\omega t) dt. \tag{10.16}$$

The quantity measured in a neutron experiment is related to the imaginary (dissipative) part of the corresponding susceptibility. It is expressed as the weighted sum of two susceptibilities: $\mathcal{S}_c(\kappa, \omega)$, which is called the coherent scattering law; and $\mathcal{S}_{ic}(\kappa, \omega)$, which is called incoherent (or single-particle) scattering law. Here $\kappa = k - k'$. The self-correlation function $G_{ic}(\mathbf{r}, t)$, introduced by Van hove, was widely used in the analysis of the incoherent scattering of slow neutrons by system of atoms of molecules; it appears also in calculations of the line shapes for resonance absorption of neutrons and gamma rays. The correlation function approach is of particular utility when the scattering system is in a nonequilibrium state: a dense gas, liquid or crystal, in which the dynamics of atomic motions are very complex. Thus, it is clear that a more sophisticated theoretical approach to the problem should be elaborated. To be able to describe the effects of retardation and dissipation properly we will proceed in a direct analogy with the derivation of the kinetic equations for a system in a thermal bath [16, 69], discussed above.

We consider a statistical medium (target) with Hamiltonian H_m, a probe (beam) with Hamiltonian H_b and an interaction V between the two $H = H_0 + V = H_m + H_b + V$. We will consider statistical medium in a nonequilibrium state. Consider the expression for the transition amplitude which describes the change of the state of the probe per unit time

$$dw(\mathbf{k} \to \mathbf{k}') = \frac{1}{\hbar^2} \int_{\infty}^{\infty} dt \mathrm{Tr}_m \Big(\rho_m(t) V_{\mathbf{k}'\mathbf{k}}(0) V_{\mathbf{k}'\mathbf{k}}(t) \Big) \exp(-i\omega t), \tag{10.17}$$

where $\rho_m(t)$ is the nonequilibrium statistical operator of target. Thus the partial differential cross-section is written in the form

$$\frac{d^2\sigma}{d\Omega dE'} = A \int_{\infty}^{\infty} \langle V(\mathbf{r}) V(\mathbf{r}', t) \rangle_m e^{[-i/\hbar(\mathbf{k}-\mathbf{k}')(\mathbf{r}-\mathbf{r}')-i\omega t]} dt d\mathbf{r} d\mathbf{r}', \tag{10.18}$$

where

$$A = \frac{m^2}{(2\pi)^3\hbar^5}\frac{k'}{k}, \quad E' = \frac{k'^2}{2m}. \tag{10.19}$$

and $\langle\ldots\rangle_m = \mathrm{Tr}_m(\rho^m(t)\ldots)$. Again, we took into account that

$$\langle\alpha'\,\mathbf{k}'|V|\alpha\,\mathbf{k}\rangle = \langle\mathbf{k}'|V(\mathbf{r})|\mathbf{k}\rangle\sum_{i=1}^{N}\langle\alpha'|e^{-\frac{i}{\hbar}(\mathbf{k}'\mathbf{R}_i)}e^{\frac{i}{\hbar}(\mathbf{k}\mathbf{R}_i)}|\alpha\rangle. \tag{10.20}$$

Thus we obtain

$$\frac{d^2\sigma}{d\Omega dE'} = \tag{10.21}$$

$$\frac{-1}{(i\hbar)^2}\tilde{A}\sum_{i,j=1}^{N}\int_0^t d\tau\sum_{\alpha}\langle\alpha|\{\exp[\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_i(\tau-t)]\exp[\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_j(0)]\exp(i\omega(\tau-t))$$

$$+\exp[\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_i(0)]\exp[\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_j(\tau-t)]\exp(-i\omega(\tau-t))\}\rho^m(t)|\alpha\rangle.$$

It can be rewritten in another form [15, 76]

$$\frac{d^2\sigma}{d\Omega dE'} = \tag{10.22}$$

$$\frac{-1}{(i\hbar)^2}\tilde{A}\sum_{i,j=1}^{N}\int_0^t d\tau\{2\mathrm{Re}\left\langle\exp[\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_i(\tau-t)]\exp[\frac{i}{\hbar}\vec{\kappa}\mathbf{R}_j(0)]\right\rangle_m\exp(i\omega(\tau-t)).$$

In terms of the density operators $n_{\vec{\kappa}} = \sum_i^N\exp(i\vec{\kappa}\mathbf{R}_i/\hbar)$ the differential cross section take the form

$$\frac{d^2\sigma}{d\Omega dE'} = \tilde{A}2\mathrm{Re}\mathcal{S}(\vec{\kappa},\omega,t), \tag{10.23}$$

where

$$\mathcal{S}(\vec{\kappa},\omega,t) = \frac{-1}{(i\hbar)^2}\int_0^t d\tau\exp[i\omega(\tau-t)]\langle n_{\vec{\kappa}}(\tau-t)n_{-\vec{\kappa}}\rangle_m, \tag{10.24}$$

Let us construct the nonequilibrium statistical operator of the medium. To do so, we should follow the basic formalism of the nonequilibrium statistical operator method. According to this approach we should take into account that

$$\rho^m = \overline{\rho_q(t,0)} = \varepsilon\int_{-\infty}^0 d\tau e^{\varepsilon\tau}\rho_q(t+\tau,\tau) =$$

$$\varepsilon\int_{-\infty}^0 d\tau e^{\varepsilon\tau}\exp\left(-\frac{H_m\tau}{i\hbar}\right)\rho_q(t+\tau,0)\exp\left(\frac{H_m\tau}{i\hbar}\right) = \varepsilon\int_{-\infty}^0 d\tau e^{\varepsilon\tau}\exp\left(-S(t+\tau,\tau)\right)(10.25)$$

Thus the nonequilibrium statistical operator of the medium will take the form

$$\rho^m(t,0) = \exp\left(-S(t,0)\right) \tag{10.26}$$

$$+\int_{-\infty}^0 d\tau e^{\varepsilon\tau}\int_0^1 d\tau'\exp\left(-\tau'S(t+\tau,\tau)\right)\dot{S}(t+\tau,\tau)\exp\left(-(\tau'-1)S(t+\tau,\tau)\right),$$

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where

$$\dot{S}(t,\tau) = \exp\left(-\frac{H_m\tau}{i\hbar}\right)\dot{S}(t,0)\exp\left(\frac{H_m\tau}{i\hbar}\right) \tag{10.27}$$

and

$$\dot{S}(t,0) = \frac{\partial S(t,0)}{\partial t} + \frac{1}{i\hbar}[S(t,0),H] = \tag{10.28}$$
$$\sum_m \left(\dot{P}_m F_m(t) + (P_m - \langle\dot{P}_m\rangle_q^t)\dot{F}_m(t)\right).$$

Finally, the general expression for the scattering function of beam of neutrons by the nonequilibrium medium in the approach of the nonequilibrium statistical operator method is given by

$$\mathcal{S}(\vec{\kappa},\omega,t) = \frac{-1}{(i\hbar)^2}\int_0^t d\tau\langle n_{\vec{\kappa}}(\tau-t)n_{-\vec{\kappa}}(0)\rangle_q^t \exp[i\omega(\tau-t)] \tag{10.29}$$
$$+\frac{-1}{(i\hbar)^2}\int_0^t d\tau \int_{-\infty}^0 d\tau' e^{\varepsilon\tau'}\left(n_{\vec{\kappa}}(\tau-t)n_{-\vec{\kappa}}(0),\dot{S}(t+\tau')\right)^{t+\tau'}\exp[i\omega(\tau-t)].$$

Here the standard notation [5] for $(A,B)^t$ were introduced

$$(A,B)^t = \int_0^1 d\tau \mathrm{Tr}\left[A\exp(-\tau S(t,0))(B-\langle B\rangle_q^t)\exp((\tau-1)S(t,0))\right], \tag{10.30}$$

$$\rho_q(t,0) = \exp(-S(t,0)); \quad \langle B\rangle_q^t = \mathrm{Tr}(B\rho_q(t,0)). \tag{10.31}$$

Now we show that the problem of finding of the nonequilibrium statistical operator for the beam of neutrons has many common features with the description of the small subsystem interacting with thermal reservoir.

Let us consider again the our Hamiltonian. The state of the overall system at time t is given by the statistical operator

$$\rho(t) = \exp\left(\frac{-iH_0t}{\hbar}\right)\rho(0)\exp\left(\frac{iH_0t}{\hbar}\right), \quad \rho(0) = \rho^m(0)\otimes\rho^b(0). \tag{10.32}$$

The initial state assumes a factorized form ($\rho^m(0)$ and $\rho^b(0)$ correspond to the density operators that represent the initial states of the system and the probe, respectively). The state of the system and the probe at time t can be described by the reduced density operators

$$\rho^b(t) = \mathrm{Tr}_m[\rho(t)] = \mathrm{Tr}_m\left(\exp(\frac{-iH_0t}{\hbar})\rho^m(0)\otimes\rho^b(0)\exp(\frac{iH_0t}{\hbar})\right), \tag{10.33}$$

$$\rho^m(t) = \mathrm{Tr}_b[\rho(t)] = \mathrm{Tr}_b\left(\exp(\frac{-iH_0t}{\hbar})\rho^m(0)\otimes\rho^b(0)\exp(\frac{iH_0t}{\hbar})\right), \tag{10.34}$$

where Tr_m and Tr_b stands for a partial trace over the system (statistical medium) and the beam (probe) degrees of freedom, respectively.

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In quantum theory a transition probability from a state of a statistical system which is described by density matrix ρ_i to the state ρ_f ("i" - initial, "f" -final) is given by

$$W_{if}(t) = \mathrm{Tr}(\rho^i(t)\rho^f(t)). \tag{10.35}$$

It is reasonable to assume that ρ^i has the form $\rho^i(t) = \rho^i(0) = |k\rangle\langle k|$. Then the transition probability per unit time takes the form

$$w_{if}(t) = \frac{d}{dt}\mathrm{Tr}(|k\rangle\langle k|\rho^f(t)) = \frac{d}{dt}\langle k|\rho^f(t)|k\rangle = \langle k|\frac{d}{dt}\rho^f(t)|k\rangle.$$

Let us consider an extended Liouville equation for the statistical medium (target) with Hamiltonian H_m, a probe (beam) with Hamiltonian H_b and an interaction V between the two. The density matrix $\rho(t)$ for the combined medium-beam complex obeys

$$\frac{\partial}{\partial t}\rho(t) - \frac{1}{i\hbar}[(H_m + H_b + V),\ \rho(t)]_- = -\varepsilon\left(\rho(t) - P\rho(t)\right). \tag{10.36}$$

Here P is projection superoperator with the properties:

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

The simplest possibility is

$$P\rho(t) = \rho^{m0}\rho^b = \rho^{m0}\sum_\alpha\langle\alpha|\rho(t)|\alpha\rangle. \tag{10.37}$$

Here ρ^{m0} is the equilibrium statistical operator of the medium.
It will be reasonable to adopt for the nonequilibrium medium the following boundary condition

$$\frac{\partial}{\partial t}\rho(t) - \frac{1}{i\hbar}[(H_m + H_b + V),\ \rho(t)]_- = -\varepsilon\left(\rho(t) - \rho^m(t)\rho^b(t)\right), \tag{10.38}$$

where

$$\rho^m(t) = \mathrm{Tr}_b(\rho(t)) = \sum_k\langle k|\rho(t)|k\rangle, \tag{10.39}$$

and (in general case)

$$\rho^b = \mathrm{Tr}_m(\rho(t)) = \sum_\alpha\langle\alpha|\rho(t)|\alpha\rangle = \sum_{kk'}\langle k'|\rho_b(t)|k\rangle|k\rangle\langle k'| = \sum_{kk'}\rho^b_{k'k}|k\rangle\langle k'|. \tag{10.40}$$

Thus, according to the nonequilibrium statistical operator method, we can rewrite Eq.(10.36) in the form

$$\frac{\partial}{\partial t}\rho(t) - \frac{1}{i\hbar}[H,\ \rho(t)]_- = -\varepsilon\left(\rho(t) - \rho^m(t)\sum_q\rho^b_{qq}(t)|q\rangle\langle q|\right), \tag{10.41}$$

where we confined ourselves to the ρ^b diagonal in states $|q\rangle$ and $(\varepsilon \to 0)$ after the thermodynamic limit. The required nonequilibrium statistical operator in accordance with Eq.(10.41) is defined as

$$\rho_\varepsilon = \rho_\varepsilon(t, 0) = \overline{\rho_q(t, 0)} = \varepsilon\int_{-\infty}^0 d\tau e^{\varepsilon\tau}\rho_q(t + \tau, \tau) = \tag{10.42}$$

$$\varepsilon\int_{-\infty}^0 d\tau U(\tau)\rho^m(t)\sum_k\rho^b_{kk}(t + \tau)|k\rangle\langle k|U^\dagger(\tau).$$

Here $U(t)$ is the operator of evolution.

In direct analogy with the derivation of the evolution equation for the small subsystem (beam) interacting with thermal reservoir (noequilibrium statistical medium) we find

$$\frac{\partial}{\partial t}\rho_{qq}^b(t) = -\frac{1}{i\hbar}\varepsilon \int_{-\infty}^{0} d\tau e^{\varepsilon\tau} \tag{10.43}$$

$$\times \sum_k \rho_{kk}^b(t+\tau) \sum_\alpha \langle\alpha|\langle q| \left[U(\tau)\rho^m(t)|k\rangle\langle k|U^\dagger(\tau), V\right]_- |q\rangle|\alpha\rangle.$$

In analogy with the derivation of the evolution equation for the small subsystem, in the lowest order approximation it is reasonably to consider that $\rho_{kk}^b(t+\tau) \simeq \rho_{kk}^b(t)$. This approximation means neglecting to the memory effects. After integration by parts we obtain the evolution equation of the form

$$\frac{\partial}{\partial t}\rho_{qq}^b(t) = \frac{1}{\hbar^2}\sum_k \rho_{kk}^b(t) \tag{10.44}$$

$$\times \int_{-\infty}^{0} d\tau e^{\varepsilon\tau} \sum_\alpha \langle\alpha|\langle q| \left[U(\tau)[V(\tau), \rho_m(t)|k\rangle\langle k|]_- U^\dagger(\tau), V\right]_- |q\rangle|\alpha\rangle.$$

As before, we confined ourselves to the second order in the perturbation V. This assumption gives also that in Eq.(10.44) $U = U^\dagger = 1$. As a result we arrive to the equation similar in the form to the equation Eq.(7.12)

$$\frac{\partial}{\partial t}\rho_{kk}^b(t) = \sum_q W_{q\to k}\rho_{qq}^b(t) - \sum_q W_{k\to q}\rho_{kk}^b(t). \tag{10.45}$$

The explicit expression for the "*effective transition probabilities*" $W_{q\to k}$ is given by the formula

$$W_{q\to k} = 2\mathrm{Re}\frac{1}{\hbar^2}\int_{-\infty}^{0} d\tau e^{\varepsilon\tau} \langle V_{qk}V_{kq}(\tau)\rangle_m^t. \tag{10.46}$$

Here $V_{qk} = \langle q|V|k\rangle$, $\langle\ldots\rangle_m^t = \mathrm{Tr}(\ldots\rho^m(t))$ and $(\varepsilon \to 0)$ after the thermodynamic limit. Thus we generalized the expressions (10.1),(10.9) and (10.17) for the nonequilibrium media. That lead to a straightforward foundation of formula (10.24) and the problem of the derivation of the Van Hove formula for scattering of neutrons on a nonequilibrium statistical medium is completed.

11   Concluding Remarks

In this paper we analyzed the foundational issues and some applications of the method of nonequilibrium statistical operator, formulated by Zubarev [5], in connection with some other approaches. By contrasting it with other methods, we tried to stress the innovative character of the NSO formalism and its internal consistency and operational ability for solving concrete problems.

To elucidate the nature of transport and relaxation processes, the generalized kinetic equations were described also for a system weakly coupled to a thermal bath [17, 69, 72]. It

was shown that the "collision term" has the same characteristic functional form as for the generalized kinetic equations for the system with small interactions among particles. The applicability of the general formalism to physically relevant situations was investigated. It was shown that some known generalized kinetic equations naturally emerges within the NSO formalism [16, 17, 18]. Relaxation of a small dynamic subsystem in contact with a thermal bath was considered on the basis of the derived equations. It is of especial interest that *the Schrödinger-type equation* for the average amplitude describing the energy shift and damping of a particle in a thermal bath and the coupled kinetic equation describing the dynamic and statistical aspects of the motion were obtained as well by this method. The equations derived can help in the understanding of quantum evolution and of the origin of irreversible behavior in quantum phenomena.

Additional material and discussion of these and related problems can be found in Refs. [15, 16, 18, 27, 28, 67, 76]

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