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Energy Conservation and the Correlation Quasi-Temperature in Open Quantum Dynamics

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Abstract: The master equation for an open quantum system is derived in the weak-coupling approximation when the additional dynamical variable—the mean interaction energy—is included into the generic relevant statistical operator. This master equation is nonlocal in time and involves the “quasi-temperature”, which is a non-equilibrium state parameter conjugated thermodynamically to the mean interaction energy of the composite system. The evolution equation for the quasi-temperature is derived using the energy conservation law. Thus long-living dynamical correlations, which are associated with this conservation law and play an important role in transition to the Markovian regime and subsequent equilibration of the system, are properly taken into account.

Keywords: open quantum system; master equation; non-equilibrium statistical operator; relevant statistical operator; quasi-temperature; dynamic correlations

1. Introduction

In this paper, we continue the study of memory effects and nonequilibrium correlations in open quantum systems, which was initiated recently in Reference [1]. In the cited paper, the nonequilibrium statistical operator method (NSOM) developed by Zubarev [2–5] was used to derive the non-Markovian master equation for an open quantum system, taking into account memory effects and the evolution of an additional “relevant” variable—the mean interaction energy of the composite system (the open quantum system plus its environment). This approach allows one to describe systematically the long-living nonequilibrium correlations associated with the total energy conservation. However, the price paid for this possibility is the need to solve the system of coupled evolution equations for the statistical operator of the open system and the additional nonequilibrium state parameters. In the present paper, our main concern is the time behaviour of the so-called quasi-temperature, which is a parameter conjugated to the mean interaction energy [1].

The structure of the paper is as follows. In Section 2, we show how a scheme for deriving master equations in open quantum dynamics can be formulated within NSOM and introduce the auxiliary “relevant” statistical operator describing correlated nonequilibrium states of the composite system. This relevant statistical operator is then used in Section 3 to derive the non-Markovian master equation in the limit of weak interaction between the open system and the environment. Nonequilibrium correlations associated with the energy conservation introduce additional relaxation terms in the master equation. These terms contain the state parameter (quasi-temperature) thermodynamically conjugated to the mean interaction energy. In Section 4, we derive the general evolution equation for the quasi-temperature and consider its modification in the weak-coupling limit. Finally, conclusions and outlook are given in Section 5.

2. The Reduced Statistical Operators and the Relevant Statistical Operator

Let us assume that the open quantum system of interest (S) interacts with another (as a rule, much larger) system (E)—the environment, and the Hamiltonian of the composite system has the form

$$H = H_S + H_E + V \equiv H_0 + V, \tag{1}$$

where H_S and H_E are the Hamiltonians of the open quantum system and the environment, and V is the interaction Hamiltonian. For the sake of simplicity, we restrict ourselves to the case when the composite system ($S + E$) is isolated and, consequently, H_S and H_E do not depend on time. It is an easy matter to generalize the main results and conclusions to the case when the open quantum system (or the environment) is affected by some alternating fields.

Nonequilibrium states of the open quantum system and the environment are completely described by the *reduced statistical operators*

$$q_S(t) = \text{Tr}_E\{q_{SE}(t)\}, \quad q_E(t) = \text{Tr}_S\{q_{SE}(t)\}, \tag{2}$$

where the symbol Tr_E (Tr_S) means the trace over all degrees of freedom of the environment (of the open quantum system), and $q_{SE}(t)$ is the statistical operator of the composite system at time t . The evolution of the composite system is described by the von Neumann equation (in units with $\hbar = 1$)

$$\frac{\partial q_{SE}(t)}{\partial t} = i[q_{SE}(t), H]. \tag{3}$$

The first step in deriving the master equation for the reduced statistical operator $q_S(t)$ is to apply the operation Tr_E to both sides of Equation (3). This gives

$$\frac{\partial q_S(t)}{\partial t} - i[q_S(t), H_S] = -i\text{Tr}_E[V, q_{SE}(t)]. \tag{4}$$

For this formal equality to have the meaning of a closed evolution equation for the subsystem (S), the statistical operator $q_{SE}(t)$ is to be expressed in terms of q_S .

Let us now consider how a scheme for deriving the master equation can be formulated within NSOM [3,4]. As usual, we start from the decomposition of the statistical operator $q_{SE}(t)$:

$$q_{SE}(t) = q_{\text{rel}}(t) + \Delta q(t), \tag{5}$$

where $q_{\text{rel}}(t)$ is the relevant part of the statistical operator for the composite system. We recall that the problem posed in NSOM is to derive evolution equations (generalized kinetic equations) for some set of observables $\langle P_i \rangle^t$ characterizing the nonequilibrium state of the system, where $\{P_i\}$ is the set of the corresponding basic dynamical variables, and the average is taken with the nonequilibrium statistical operator of the system (in the present case with $q_{SE}(t)$). The problem now is to construct a proper relevant statistical operator that is a functional of the observables. It is commonly required that $q_{\text{rel}}(t)$ corresponds to the extremum of the information entropy $S(t) = -\text{Tr}_{S,E}\{q_{\text{rel}}(t) \ln q_{\text{rel}}(t)\}$ under the supplementary conditions that the mean values $\langle P_i \rangle^t$ be equal to given quantities and the normalization condition $\text{Tr}_{S,E}\{q_{\text{rel}}(t)\} = 1$. Under these conditions we have [3]

$$q_{\text{rel}}(t) = \exp\left\{-\Phi(t) - \sum_i F_i(t)P_i\right\}. \tag{6}$$

The Massieu-Planck function $\Phi(t)$ is determined by normalization,

$$\Phi(t) = \ln \text{Tr} \exp \left\{ - \sum_i F_i(t) P_i \right\}, \tag{7}$$

where the parameters $F_i(t)$ (Lagrange multipliers) are found from the self-consistency conditions

$$\langle P_i \rangle^t = \text{Tr} \{ P_i \rho_{\text{rel}}(t) \}, \tag{8}$$

which can be considered as the nonequilibrium equations of state.

The answer to which set of the dynamic variables P_i is preferable depends on the kind of the system and the required level of its description. For instance, the “hydrodynamic” description corresponds to taking the densities of conserved quantities as a basic set of the dynamical variables [4]. An extension of this set at the expense of higher derivatives allows one to obtain equations of the generalized hydrodynamics and to widen the timescale of the description of the system evolution. Such a scheme underlies the generalized collective mode theory (GCM) [6–8], which has proven its efficiency at the study of variety of the condensed matter systems.

Conversely, the GCM can be extended by taking into account the “ultraslow” processes (defined by the time integrals of corresponding densities) [9–11]), which allows one to approach the problems of account for slow structural relaxation and study the ageing processes in the glassy forming system on equal footing with the extended hydrodynamics [12].

Thus, the main criterion for the choice of the dynamic variables of the abbreviated description of the system is a slowness of their variation on the chosen time scale. A closer examination of this point is given, e.g., in the books [2–4]. Leaving aside the problems connected with initial correlations, memory effects, and other special features of quantum dynamics, for a moment, we will consider the fundamental question about the possibility of deriving a master equation for an open quantum system within the framework of NSOM. The problem is to find dynamical variables P_i such as their mean values, calculated with the statistical operator $\rho_{SE}(t)$, contain the same information about the state of the open system (S) as the reduced statistical operator $\rho_S(t)$.

To this end, let us consider some complete and orthonormal set $\mathcal{G} = \{|n\rangle\}$ of quantum states in the Hilbert space of the open system (S). We introduce the so-called *Hubbard operators* [13]

$$X_{mn} = |m\rangle\langle n|, \tag{9}$$

which obey the following algebraic properties:

$$X_\alpha X_{\alpha'} = \sum_{\alpha''} g_{\alpha\alpha';\alpha''} X_{\alpha''}, \quad [X_\alpha, X_{\alpha'}] = \sum_{\alpha''} c_{\alpha\alpha';\alpha''} X_{\alpha''} \tag{10}$$

with the structure constants

$$g_{\alpha\alpha';\alpha''} = \delta_{mm''} \delta_{nm'} \delta_{n'n''}, \quad c_{\alpha\alpha';\alpha''} = g_{\alpha\alpha';\alpha''} - g_{\alpha'\alpha;\alpha''}. \tag{11}$$

To simplify some notations, we have introduced the ordered pairs of indexes $\alpha = (m, n)$, $\alpha' = (m', n')$, etc.

Let us show that the matrix elements of the reduced statistical operator $\rho_S(t)$ of the open system (S) are expressed in terms of the mean values $\langle X_{mn} \rangle^t$, where the averaging is performed with the statistical operator of the composite system ($S + E$). To do this we write the obvious chain of equalities:

$$\langle X_{mn} \rangle^t \equiv \text{Tr}_{SE} \{ X_{mn} \rho_{SE}(t) \} = \text{Tr}_S \{ X_{mn} \rho_S(t) \} = \sum_{k,k'} \langle k | X_{mn} | k' \rangle \langle k' | \rho_S(t) | k \rangle, \tag{12}$$

where relation (2) has been used. Since, in calculating the trace, we may take $|k\rangle \in \mathcal{G}$ and $|k'\rangle \in \mathcal{G}$, it follows from the definition (9) that $\langle k|X_{mn}|k'\rangle = \delta_{km}\delta_{k'n}$. Consequently,

$$\langle X_{mn} \rangle^t = \langle n|q_S(t)|m \rangle. \tag{13}$$

Thus, there is a good reason to include the Hubbard operators into the basic set of dynamical variables $\{P_i\}$. Such an approach was used, for instance, in Reference [14] to study the role of initial correlations for a system consisting of many two-level atoms interacting with a common bath.

Before writing down the explicit form of the relevant statistical operator, we would like to emphasize that the first term appearing in Equation (5) is by itself an auxiliary operator, but it plays an important role in NSOM. First, the choice of the relevant statistical operator determines the initial (or boundary) condition for $\Delta\rho(t)$ (see, e.g., Ref. [1]). Second, the choice of $q_{\text{rel}}(t)$ determines the “structure” of approximations in solving the von Neumann Equation (3), since the scheme of NSOM works most effectively when the operator $\Delta\rho(t)$ may in a sense be regarded as a small correction to the relevant part of the statistical operator (5).

To be sure that all slow variables are incorporated in the relevant statistical operator, let us recall that regardless of the structure of the open system and the properties of the environment, there is the quantity (namely the average energy of the composite system $\langle H \rangle^t$) which does not depend on time and, consequently, is “slowly varying” at all time scales. As shown in Reference [15], taking into account the energy conservation changes drastically the structure of non-Markovian kinetic equations even in the Born approximation and ensures the existence of the equilibrium solution for the statistical operator. Within NSOM, the additional “correlational” terms appearing in a kinetic equation can be found in an explicit form, if $\langle H \rangle^t$ is included into the set of observables to construct the relevant statistical operator. It is often convenient to take as a controlled parameter of state not the total energy of the system but the mean interaction energy since all the remaining contributions to $\langle H \rangle^t$ can be obtained by redefining the Lagrange multipliers for other basic dynamical variables [15].

Following Reference [1], we take the relevant statistical operator of the composite system in the form

$$q_{\text{rel}}(t) = \exp \left\{ -\Phi(t) - \sum_{\alpha} \Lambda_{\alpha}(t) X_{\alpha} - \beta^*(t) V - \beta H_E \right\}. \tag{14}$$

As usual, the Massieu-Planck function is determined from the normalization condition for the operator $q_{\text{rel}}(t)$, and the Lagrange multipliers $\Lambda_{\alpha}(t)$, $\beta^*(t)$ are determined from the self-consistency conditions

$$\text{Tr}_{SE} \{ X_{\alpha} q_{\text{rel}}(t) \} = \langle X_{\alpha} \rangle^t, \quad \text{Tr}_{SE} \{ V q_{\text{rel}}(t) \} = \langle V \rangle^t, \tag{15}$$

where the averages $\langle X_{\alpha} \rangle^t$ and $\langle V \rangle^t$ are calculated with the nonequilibrium statistical operator $q_{SE}(t)$ of the composite system.

The relevant statistical operator (14) has some important properties. For example, if we set $\beta^* = \beta$, then q_{rel} coincides with the exact equilibrium statistical operator at temperature $T = (k_B\beta)^{-1}$. In this connection, the quantity $T^* = (k_B\beta^*)^{-1}$ may be interpreted as a *correlational quasi-temperature* of the open system. On the other hand, if we put $\beta^* = 0$ (or $T^* = \infty$), then the relevant statistical operator (14) describes the state in which there are no correlations between the open system and the environment,

$$q_{\text{rel}}^{(0)}(t) = \exp \left\{ -\Phi^{(0)}(t) - \sum_{\alpha} \Lambda_{\alpha}(t) X_{\alpha} - \beta H_E \right\}. \tag{16}$$

This expression can be cast into the form

$$\rho_{\text{rel}}^{(0)}(t) = \rho_S(t) \otimes \rho_E, \tag{17}$$

where

$$\rho_E = \exp\{-\Phi_E^{(0)} - \beta H_E\} \tag{18}$$

is the equilibrium statistical operator of the environment, and the statistical operator of the subsystem S is defined as

$$\rho_S(t) = \exp\left\{-\Phi_S^{(0)}(t) - \sum_{\alpha} \Lambda_{\alpha}(t) X_{\alpha}\right\}. \tag{19}$$

As above, the Massieu-Planck function $\Phi_S^{(0)}(t)$ is determined from the normalization condition for the operator on the left-hand side.

The relevant statistical operator (16) can be used to determine the initial condition $\rho_{SE}(0) = \rho_{\text{rel}}^{(0)}(0)$ if the evolution of the composite system starts from a non-correlated state. However, even in this simplest case, for all times—not just at time $t = 0$ —the absence of correlations is not true and consequently nonequilibrium states are not adequately described by statistical operator (16).

3. The Weak-Coupling Master Equation

Starting from the description of nonequilibrium states of the composite system by the relevant statistical operator (14), one can derive the master equation for $\rho_S(t)$. To explain the scheme of the derivation, we shall consider the case where the operator V in the Hamiltonian (1) describes weak interaction between the open quantum system and the environment, i.e., it is possible to expand at some stage the quantities of interest in a power series in the coupling constant to which the operator V is proportional.

First we substitute the expression (5) into Equation (4):

$$\frac{\partial \rho_S(t)}{\partial t} - i[\rho_S(t), H_S] = -i\text{Tr}_E[V, \rho_{\text{rel}}(t)] - i\text{Tr}_E[V, \Delta \rho(t)]. \tag{20}$$

Now, following the logic of NSOM, the operator $\Delta \rho$ is to be expressed in terms of ρ_{rel} . Then the right-hand side of Equation (20) could, in principle, be considered as a functional of ρ_S and β^* . For this purpose, we first derive the evolution equation for the operator $\Delta \rho(t)$. Let us substitute the expression (5) into the von Neumann Equation (3) and then change to the interaction picture by setting

$$\tilde{A}(t) = e^{itH_0} A(t) e^{-itH_0} \tag{21}$$

for any operator $A(t)$. After simple manipulations we obtain

$$\frac{\partial}{\partial t} \Delta \tilde{\rho}(t) - i[\Delta \tilde{\rho}(t), \tilde{V}(t)] = -\left(\frac{\partial}{\partial t} \tilde{\rho}_{\text{rel}}(t) - i[\tilde{\rho}_{\text{rel}}(t), \tilde{V}(t)]\right). \tag{22}$$

Let us assume that the initial condition $\Delta \tilde{\rho}(0) = \Delta \rho(0) = 0$ is satisfied. It means that the evolution of the composite system starts from the state characterized by the condition $\rho_{SE}(0) = \rho_{\text{rel}}(0)$. This is typical when the open quantum system is prepared in a particular way (e.g., by some quantum measurement [16]). Then Equation (22) can be written in the integral form

$$\Delta \tilde{\rho}(t) - i \int_0^t d\tau [\Delta \tilde{\rho}(\tau), \tilde{V}(\tau)] = - \int_0^t d\tau \left(\frac{\partial}{\partial \tau} \tilde{\rho}_{\text{rel}}(\tau) - i[\tilde{\rho}_{\text{rel}}(\tau), \tilde{V}(\tau)]\right). \tag{23}$$

If the interaction between the open subsystem and its environment is weak, then, as is clear from Formula (20), in the leading (Born) approximation it is sufficient to calculate $\Delta q(t)$ up to terms linear in V . Apparently, in this approximation the second term on the left-hand side of Equation (23) may be omitted. Using interaction representation (21) once again, we obtain

$$\Delta q(t) = - \int_0^t d\tau e^{-i(t-\tau)H_0} \left(\frac{\partial q_{\text{rel}}(\tau)}{\partial \tau} - i[q_{\text{rel}}(\tau), H] \right) e^{i(t-\tau)H_0}. \tag{24}$$

The commutator in (24) is transformed in a standard way using definition (14) for the relevant statistical operator, the Kubo identity for non-commuting operators [3] and the self-consistency conditions (15). As a result, up to terms linear in V , we have

$$\Delta q(t) = -i \int_0^t d\tau e^{-i(t-\tau)H_0} R(\tau) e^{i(t-\tau)H_0}, \tag{25}$$

where

$$R(\tau) = [V, \varrho_S(\tau) \varrho_E] + \beta^*(\tau) \int_0^1 dx (\varrho_S(\tau) \varrho_E)^x [V, H_0] (\varrho_S(\tau) \varrho_E)^{1-x}. \tag{26}$$

In Equation (26) the superscript, which emerges due to the Kubo identity, denotes the x -th power of the corresponding statistical operators.

Using Formula (25), we can bring Equation (20) to its final form

$$\frac{\partial \varrho_S(t)}{\partial t} - i[q_S(t), H_S] = -i \text{Tr}_E [V, \varrho_{\text{rel}}(t)] - \int_0^t d\tau \text{Tr}_E [V, e^{-i(t-\tau)H_0} R(\tau) e^{i(t-\tau)H_0}]. \tag{27}$$

It follows from the above analysis that both terms on the right-hand side of this equation are functionals of $\varrho_S(t')$ and $\beta^*(t')$, where $0 < t' \leq t$. However, Equation (27) is not itself a closed master equation for the reduced statistical operator ϱ_S because we need also the evolution equation for $\beta^*(t)$ or for the correlational quasi-temperature $T^*(t) = (k_B \beta^*(t))^{-1}$. A similar situation arises in the “standard” kinetic theory when nonequilibrium correlations are taken into account in non-Markovian kinetic equations. Within the weak coupling approximation, the equation for $\beta^*(t)$ was derived in the work [15] where a quantum system of particles with pair interaction was considered. As already noted, the approach to the dynamics of open systems presented here is formally quite analogous to NSOM in quantum kinetics, so that the equation for $\beta^*(t)$ can be derived by applying the scheme described in the work [15].

4. Equation for the Quasi-Temperature

Let us turn to the self-consistency conditions (15) and differentiate them with respect to time. Recalling the explicit form (14) of the relevant statistical operator and the definition (7) of the Massieu-Planck function leads to the set of equations

$$\begin{cases} (X_\alpha, V) \frac{d\beta^*(t)}{dt} + \sum_{\alpha'} (X_\alpha, X_{\alpha'}) \frac{d\Lambda_{\alpha'}(t)}{dt} = - \frac{d\langle X_\alpha \rangle^t}{dt}, \\ (V, V) \frac{d\beta^*(t)}{dt} + \sum_{\alpha} (V, X_\alpha) \frac{d\Lambda_\alpha(t)}{dt} = - \frac{d\langle V \rangle^t}{dt}. \end{cases} \tag{28}$$

We have introduced the time-dependent correlation functions of dynamical variables in the relevant ensemble,

$$(A, B) = \int_0^1 dx \langle \Delta A \varrho_{\text{rel}}^x \Delta B \varrho_{\text{rel}}^{-x} \rangle_{\text{rel}}, \quad \Delta A = A - \langle A \rangle_{\text{rel}}^t, \tag{29}$$

where $\langle \dots \rangle_{\text{rel}} \equiv \text{Tr}_{S,E} \{ \varrho_{\text{rel}}(t) \dots \}$ denotes averaging with the relevant statistical operator (14). It is easy to check that the correlation function (29) satisfies the symmetry condition $(A, B) = (B, A)$.

The chain of matrix Equations (28) can formally be solved for the derivatives $d\Lambda_\alpha(t)/dt$, yielding the evolution equation for the quasi-temperature:

$$C(t) \frac{d\beta^*(t)}{dt} = \sum_{\alpha, \alpha'} (V, X_\alpha) (X, X)_{\alpha\alpha'}^{-1} \frac{d\langle X_{\alpha'} \rangle^t}{dt} - \frac{d\langle V \rangle^t}{dt}, \tag{30}$$

where (X, X) is a matrix whose elements are $(X_\alpha, X_{\alpha'})$, and the quantity

$$C(t) = (V, V) - \sum_{\alpha, \alpha'} (V, X_\alpha) (X, X)_{\alpha\alpha'}^{-1} (X_{\alpha'}, V) \tag{31}$$

may be regarded as a generalized heat capacity.

Let us rewrite the right-hand side of Equation (30) in a more transparent form. First we eliminate the derivative $d\langle V \rangle/dt$ applying the energy conservation law

$$\frac{d\langle H_S \rangle^t}{dt} + \frac{d\langle H_E \rangle^t}{dt} + \frac{d\langle V \rangle^t}{dt} = 0, \tag{32}$$

and then express the derivative $d\langle H_S \rangle/dt$ in terms of $d\langle X_\alpha \rangle/dt$ using the fact that, in general, the system Hamiltonian H_S can be written as

$$H_S = \sum_{\alpha} \mathcal{E}_{\alpha} X_{\alpha} \tag{33}$$

with $\mathcal{E}_{\alpha} \equiv \mathcal{E}_{mn} = \langle m | H_S | n \rangle$. After the above manipulations, Equation (30) takes the form

$$C(t) \frac{d\beta^*(t)}{dt} = \sum_{\alpha} \left(\mathcal{E}_{\alpha} + \sum_{\alpha'} (V, X_{\alpha'}) (X, X)_{\alpha'\alpha}^{-1} \right) \frac{d\langle X_{\alpha} \rangle^t}{dt} + \frac{d\langle H_E \rangle^t}{dt}. \tag{34}$$

For the time derivatives on the right-hand side of this equation, we have the expressions

$$\begin{aligned} \frac{d\langle X_{\alpha} \rangle^t}{dt} &= -i \langle [X_{\alpha}, H_S] \rangle_S^t - i \langle [X_{\alpha}, V] \rangle_{\text{rel}}^t + I_{\alpha}(t), \\ \frac{d\langle H_E \rangle^t}{dt} &= -i \langle [H_E, V] \rangle_{\text{rel}}^t + I_E(t), \end{aligned} \tag{35}$$

where $\langle \dots \rangle_S^t$ means averaging with the reduced statistical operator $\varrho_S(t)$, and

$$I_{\alpha}(t) = -i \text{Tr}_{S,E} \{ [X_{\alpha}, V] \Delta \varrho(t) \}, \quad I_E(t) = -i \text{Tr}_{S,E} \{ [H_E, V] \Delta \varrho(t) \}. \tag{36}$$

Formulas (35) follow directly from the von Neumann Equation (3) and Equation (5).

Let us show that the first term on the right-hand side of the evolution Equation (35) for $\langle H_E \rangle^t$ is equal to zero. To this end, we use the obvious identity

$$\text{Tr}_{S,E} \{ \varrho_{\text{rel}}(t) [A, \ln \varrho_{\text{rel}}(t)] \} = 0, \tag{37}$$

which is valid for any operator A . Taking $A = H_E$ and recalling the explicit form (14) of the relevant statistical operator, one readily obtains

$$\text{Tr}_{S,E} \{ \varrho_{\text{rel}}(t) [H_E, V] \} = 0. \tag{38}$$

Substituting Equation (35) into Equation (34) leads, in general, to a rather cumbersome evolution equation for the quasi-temperature. However, this equation can be considerably simplified, if the system-environment coupling is weak. To do this, let us assume that $\langle V \rangle_E \equiv \text{Tr}_E (V \varrho_E) = 0$, where ϱ_E is given by Equation (18). If the initial operator V does not satisfy this condition, then it suffices to redefine H_S and V by replacing $H_S \rightarrow H_S + \langle V \rangle_E$ and $V \rightarrow V - \langle V \rangle_E$. Then it is easy to check that the leading terms in the correlation functions $\langle X_{\alpha'} V \rangle$ as well as in the mean values $\langle [X_{\alpha'}, H_S] \rangle_{\text{rel}}^t$ are of the second order in interaction. In this approximation, Equation (34) reduces to

$$C(t) \frac{d\beta^*(t)}{dt} = -i \sum_{\alpha} \left\{ \mathcal{E}_{\alpha} \langle [X_{\alpha}, V] \rangle_{\text{rel}}^t + \sum_{\alpha'} (V, X_{\alpha'}) (X, X)_{\alpha'\alpha}^{-1} \langle [X_{\alpha}, H_S] \rangle_S^t \right\} + \sum_{\alpha} \mathcal{E}_{\alpha} I_{\alpha}(t) + I_E(t), \tag{39}$$

where the generalized heat capacity $C(t)$ is to be evaluated with the relevant statistical operator (16) for a non-interacting composite system. This gives

$$C(t) = \int_0^1 dx \text{Tr}_{S,E} \left\{ V \left(\varrho_{\text{rel}}^{(0)} \right)^x V \left(\varrho_{\text{rel}}^{(0)} \right)^{1-x} \right\}. \tag{40}$$

Note that the time dependence of the generalized heat capacity (40) arises from that of the relevant statistical operator (16).

We would like to note that the ‘‘coherent’’ term $\sum_{\alpha} \mathcal{E}_{\alpha} \langle [X_{\alpha}, H_S] \rangle_S^t$ in Equation (39) vanishes due to Equation (33). It can also be shown that within the leading weak coupling approximation the term in braces in Equation (39) vanishes, so that we finally arrive at the simplified equation for the quasi-temperature:

$$C(t) \frac{d\beta^*(t)}{dt} = \sum_{\alpha} \mathcal{E}_{\alpha} I_{\alpha}(t) + I_E(t). \tag{41}$$

Let us touch upon a physical meaning of the quasi-temperature in more detail. Of course, $1/\beta^*(t)$ cannot be treated as a temperature in its ordinary meaning since it cannot be even measured. Moreover, the quasi-temperature can even be negative if the system admits the dynamically induced inversion of the levels’ population [17–19]. However, $1/\beta^*(t)$ can really be considered as the generalized temperature since: (i) it is introduced in a quasi-Gibbsian manner via the relevant statistical operator similarly (14), like the ordinary temperature is; (ii) it obeys the generalized thermodynamic relation (41), whose right-hand side is nothing but the derivative of the total kinetic energy of the composite ($S + E$) system; (iii) it tends to its asymptotic value at $t \rightarrow \infty$ [20], which coincides with the bath temperature.

To conclude this Section, and to explain the essence and the importance of the dynamical correlations in more detail we would like to note the following. The dynamical correlations are incorporated in the master Equation (27) by means of the second term of (26), which involves the quasi-temperature $1/\beta^*(t)$. First, the quasi-temperature is defined as the state parameter

conjugated to the interaction energy, see definition (14) of the relevant statistical operator. On the other hand, the dynamic equation (41) for the quasi-temperature involves both the generalized heat capacity (40) (which is expressed in terms of the “energy-energy” non-equilibrium correlation functions), and collision integrals (36) (which also bring the information about the dynamical correlations between the system and environment arising from the conservation law (32)).

Moreover, the second term in Equation (26) gives rise to additional contributions to the collision integrals $I_S(t)$ and $I_E(t)$ by taking the non-equilibrium correlations into account. These terms are even called “correlational” ones [3,15,21], and they determine an additional relaxation timescale [20], which turns out to be much shorter than that of the (S) subsystem dynamics.

5. Conclusions and Outlook

Equation (41) for the quasi-temperature and the master Equation (27) for the reduced statistical operator provide us with a complete description of open quantum dynamics in the weak coupling limit. It must be emphasized that both equations are non-local in time due to the structure of the nonequilibrium correction $\Delta\rho(t)$ to the statistical operator (see Equation (25)).

Note that the interplay between memory effects and correlations may strongly affect kinetic processes [15,21]. First of all, a transition to the Markovian regime (when the memory effects become negligible) occurs due to the energy conservation and the long-living dynamical correlations, accompanying this phenomenon. It is known [3] that the Levinson equation (non-Markovian one) does not have an equilibrium solution, while the local in time Uehling-Uhlenbeck equation does. The correlational term eliminates this bottleneck of the quantum kinetic theory by providing a proper Markovization of the system and tending of the distribution functions to their (quasi)equilibrium limits. At this stage of the system evolution, the quasi-temperature $1/\beta^*(t)$ tends to its equilibrium value $1/\beta$, both correlational parts of the collision integrals (36) and Equation (41) become identically equal to zero, and the non-Markovian quantum kinetic equation converts to its Uehling-Uhlenbeck form.

From a strictly mathematical point of view, the time non-locality (non-Markovian effects) appears at the stage of integral presentation of the von Neuman equation regardless of taking the dynamical correlations into account. It means that the master Equation (27) turns out to be non-Markovian even if one neglects the second term in (26). Though the Markovian approximation is widely believed [16] to be justified if the time scale τ_S , over which the state of the system varies appreciably, is large compared to the time scale τ_E , over which the environment correlation functions decay, in the case of a particular open quantum system the situation can be more diverse. One can formally solve the (Heisenberg) equations of motions for the environment variables and insert the obtained results into the dynamic equations for the (S) subsystem variables. The obtained Langevin-type equations are found to be non-Markovian. However, if the dynamics of the environment variables is not strongly interconnected with that of the (S) subsystem, and the time behaviour of the bath variables can be calculated explicitly, one comes to the Markovian kinetic equations without any suggestions about relaxation times hierarchy. This is exactly the case of the dephasing model [22], where the dynamic equation for the system coherency does not involve the memory effects.

Secondly, memory effects are most pronounced at the initial stage of the system dynamics. In particular, their consideration turns out to be indispensable in the presence of ultra-short external fields [20]. Similar situations in which memory effects and correlations play an important role can emerge in open quantum systems. For instance, the period between switching of quantum registers can be comparable or even less than the dephasing time [22].

Finally, there exist various approaches [23–25] to the quantification of memory effects in quantum open systems, and even to the definition (or redefinition) of the non-Markovianity itself. Usually, they are based upon a conception of the trace distance between two quantum states, and the obtained

results are expressed in terms of the rate of change of the above mentioned distance. In this context, one can propose another look at this issue, which is based, say, on the concept of the generalized thermodynamics. In particular, one can investigate the transition times from the essentially non-Markovian regimes to the local in time dynamics (which would manifest itself in tending of the quasi-temperature to its equilibrium limit) and compare them with other typical timescales for open quantum systems (e.g., the dephasing time or the thermalization time [22]). The ratio between the above mentioned times can be treated as a generalized measure of the non-Markovianity. In our opinion, such an approach would be most promising for small-sized systems, when the environment can hardly be treated as a thermal bath. It should be noted that our scheme can be directly applied to this case, when the environment has not been equilibrated yet and is characterized by the non-equilibrium temperature $1/\beta(t)$ which, in general, is not equal to the “correlational” quasi-temperature $1/\beta^*(t)$.

Definitely, the consistency and the robustness of our scheme should be verified on particular models of the open quantum systems. We believe these studies to be very perspective, and we are going to carry them out in our further researches using some exactly solvable models.

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