Master equation – tutorial approach

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Abstract

We do not present any original or new material. This is a tutorial addressed to students who need to study the microscopic derivation of the quantum-mechanical master equation encountered in many practical physical situations.

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1 Introduction

1.1 Motivation

The term "master equation" (ME) used in this work means an equation of motion for the reduced density operator $\rho_A(t)$ of subsystem $A$ which interacts with (usually much larger) another subsystem $B$. Experiences gathered during quite a few years of lecturing indicate that students find it difficult to understand the derivation and consequences of ME. The literature sources (at least those known to us) are usually quite brief and not easy to follow.

The aim of this paper is to give a full presentation of the so-called microscopic derivation of ME together with detailed discussion of the underlying assumptions and approximations. Hence, this work does not bring any original material. It is just a tutorial which, hopefully, will help the students to obtain a better grasp of the ideas and concepts leading to one of important theoretical methods used in a variety of physical problems.

The literature of the subject is quite rich. Entering the term "master equation" into Google Scholar returns about 30 000 links. It seems virtually impossible to give an extensive bibliography. Therefore, we concentrate only on several works which were essential in the preparation of this paper.

1.2 Outline of the problem

In order to present the ME technique, we first give the basic ideas which help, so to speak, to set the scene for further developments. We assume that the reader is familiar with fundamental concepts of quantum mechanics (given, for example, in the main chapters of the first volume of the excellent book by Cohen-Tannoudji et al [1]).

To start with, we recall that the state of the quantum system is, in the majority of practical applications, given by the density operator. This concept is introduced and discussed in virtually all handbooks on quantum mechanics, hence we mention only the basic facts which will be needed here. Namely, density operator for any physical system must have three essential properties

$$
\rho = \rho^\dagger, \quad \text{hermiticity;}
$$

$$
\text{Tr}\{\rho\} = 1, \quad \text{normalization;}
$$

$$
\rho \geq 0, \quad \text{semi-positivity.}
$$

The last inequality means that $\langle \psi | \rho | \psi \rangle \geq 0$ for any state $|\psi\rangle$ from the Hilbert space of the states of the given physical system. These properties may be phrased in terms of the eigenvalues $\lambda_k$ of the density operator. Namely, $\lambda_k \in \mathbb{R}$, $\sum_k \lambda_k = 1$, and $\lambda_k \geq 0$.

For a closed system with hamiltonian $H$, the evolution of the corresponding density operator is given by the von Neumann equation

$$
ih \frac{d}{dt} \rho(t) = \left[ H, \rho(t) \right],
$$

(2)
which has a well-known solution

$$\rho(t) = U(t,t_0) \rho(t_0) U^*(t,t_0), \quad \text{with} \quad U(t,t_0) = \exp \left( -\frac{i}{\hbar} H(t-t_0) \right),$$

(3)

where $\rho(t_0)$ is a suitably chosen initial condition. Such an evolution is unitary \(^1\) and obviously preserves all the necessary properties \(^{11}\) of the density operator. In such a case everything is conceptually clear although necessary calculation may be quite involved or even requiring some approximate computational methods.

The problem arises when we deal with a bipartite system $A+B$, consisting of two interacting subsystems $A$ and $B$. Let us briefly outline the physical situation. We assume that the whole system $A+B$ is closed and the total hamiltonian is written as

$$H_{AB} = H_0 + V_{AB}, \quad \text{where} \quad H_0 = H_A \otimes 1_B + 1_A \otimes H_B,$$

(4)

where $H_A$ and $H_B$ are free, independent hamiltonians of each of the subsystems $A$ and $B$. $V_{AB}$ is the hamiltonian describing the interaction between two parts. Let $\rho_{AB}(t)$ denote the density operator of the total system. Then, $\rho_{AB}(t)$ evolves according to the von Neumann equation (identical as (2))

$$i \hbar \frac{d}{dt} \rho_{AB}(t) = \left[ H_{AB}, \rho_{AB}(t) \right],$$

(5)

Now, one may ask, what is the problem? The point is that we are, in fact, interested only in the subsystem $A$. Subsystem $B$, for this reason or other, is considered irrelevant, although the $A$-$B$ interaction certainly affects the evolution of $A$. Moreover, in many practical cases, subsystem $B$ is much larger (with many more degrees of freedom) and virtually inaccessible to direct measurements. Frequently, $B$ is a reservoir \(^2\), \(^3\) and plays the role of environment upon which we have neither control nor influence. This may be very important in the context of quantum information theory \(^4\), \(^5\) when the relevant subsystem is disturbed by the surroundings. Moreover, problems of decoherence and irreversibility are intrinsically connected with the effects occurring in a subsystem influenced by an external reservoir (see \(^3\), \(^4\)). We shall not discuss these problems but focus on master equation technique.

In the view of these brief remarks the question is, how to extract useful information on $A$ from the general von Neumann equation (5). We stress that we are interested only in system $A$, so we need to find the reduced density operator

$$\rho_A(t) = \text{Tr}_B\{\rho_{AB}(t)\}.$$  

(6)

The aim is, therefore, twofold:

(i) extract the evolution of $\rho_A(t)$ from Eq. (5) for the entire system $A+B$.

(ii) do it in a way which guarantees that properties $^{11}$ of $\rho_A(t)$ (as of any density operator) are preserved for any moment of time.
The solution to the stated problems is found in the so-called master equation technique. There are two, conceptually different but complementary, approaches to ME.

The first one uses mathematically rigorous methods. Such an approach is presented, for example, in Refs. [2, 3] (see also the references given in these books). Rigorous mathematics is obviously very important from the fundamental point of view. Mathematical theorems prove that ME for the reduced density operator of subsystem $A$ follows from general von Neumann equation (5) and indeed preserves properties (1). In Refs. [2, 3, 4] it is shown that it is so, when ME attains the so-called standard (Lindblad-Gorini-Kossakowski-Sudarshan) form (Ref. [2], p.8, Eq. (38); [3], Eq. (3.63) and [4], Eq. (78))

$$\frac{d}{dt} \rho_A(t) = \frac{1}{i\hbar} [H, \rho_A(t)] + \sum_{ij} a_{ij} \left( F_i \rho_A(t) F_i^\dagger - \frac{1}{2} [F_i^\dagger F_i, \rho_A(t)]_+ \right). \quad (7)$$

The first term leads the unitary (hamiltonian) evolution, while the second one is sometimes called a dissipator [3]. Operators $F_i$ constitute a basis in the space of operators for $A$ subsystem (see [2, 3]). Finally, $a_{ij}$ is a positive definite hermitian matrix. Here, we do not go into the details of the derivation of the standard form (7) of the master equation, we refer the reader to the mentioned references (see also [4]). Quite interesting derivation of standard ME is given by Preskill [5]. His presentation is somewhat heuristic but certainly worth reading, especially if one is interested in connection with quantum information theory, quantum channels etc. It is not, however, our aim to pursue formal mathematical issues. Our intentions are quite practical, so the reader may ask, why do we speak about the standard form of ME. The reason is as follows.

The second approach to the stated problems is via "microscopic derivations". This occurs when we need to consider a specific physical situation when interacting systems $A$ and $B$ are known and well-defined. Then, we want to construct the corresponding ME – equation of motion for the reduced density operator $\rho_A(t)$. This is less formal and may be mathematically uncertain. If the microscopic derivation yields an equation in the standard form (7), we can say that the aim is achieved, because standard form ensures the preservation of the necessary properties of reduced density operator $\rho_A(t)$. Hence, both approaches are complementary. Formal but rigorous mathematical methods lead to standard form of ME which must be matched by equations obtained through microscopic derivation.

All of the already mentioned references give (usually brief) account on the microscopic derivation of ME. These presentations seem to be difficult for students who are not acquainted with the subject and who seek the necessary introduction. Perhaps the most extensive microscopic derivation is given by Cohen-Tannoudji, Dupont-Roc and Grynberg [6]. This latter presentation is somewhat heuristic and, as it seems to us, leaves some nuances unexplained. There is, however, one more drawback. Namely, Cohen-Tannoudji et al do not compare their ME with the standard form. Therefore, essential question of positivity preservation remains untouched.
2 Evolution of the reduced density operator

2.1 Introductory remarks

We consider a physical system which consists of two parts $A$ and $B$. We are interested only in what happens in part $A$ which is usually much smaller than part $B$. The latter one we will call a reservoir (environment). We assume that the entire system $A + B$ is closed. Then, its Hamiltonian is specified as in Eq. (4). Some additional assumptions concerning both subsystems will be introduced when necessary.

A previously, let $\rho_{AB}(t)$ denote the density operator of the whole system $A + B$. The evolution of this operator is governed by von Neumann equation (5). Our main aim is to find the corresponding equation of motion for the reduced density operator $\rho_A = \text{Tr}_B{\rho_{AB}}$ for the subsystem $A$. Our starting point is provided by von Neumann equation which, after the transformation to the interaction picture, reads

$$\frac{d}{dt} \tilde{\rho}_{AB}(t) = \frac{1}{i\hbar} \left[ \tilde{V}_{AB}(t), \tilde{\rho}_{AB}(t) \right],$$

where, we obviously denoted

$$\tilde{\rho}_{AB}(t) = e^{iH_0t/\hbar} \rho_{AB}(t) e^{-iH_0t/\hbar}, \quad \tilde{V}_{AB}(t) = e^{iH_0t/\hbar} V_{AB} e^{-iH_0t/\hbar},$$

with $H_0$ given in Eq. (4). Reduction of the density operator (as in $\rho_A = \text{Tr}_B{\rho_{AB}}$) for the subsystem $A$. Our starting point is provided by von Neumann equation which, after the transformation to the interaction picture, reads

$$\tilde{\rho}_A(t) = \text{Tr}_B{\tilde{\rho}_{AB}(t)}. \quad (10)$$

Formal integration of Eq. (8) yields the following expression

$$\tilde{\rho}_{AB}(t + \Delta t) = \tilde{\rho}_{AB}(t) + \frac{1}{i\hbar} \int_t^{t+\Delta t} dt_1 \left[ \tilde{V}_{AB}(t_1), \tilde{\rho}_{AB}(t_1) \right],$$

with $\Delta t$ given in Eq. (4).
which gives the density operator at a later moment \( t + \Delta t \), while the initial one at a moment \( t \) is assumed to be known. Iterating further and denoting

\[
\Delta \tilde{\rho}_{AB}(t) = \tilde{\rho}_{AB}(t + \Delta t) - \tilde{\rho}_{AB}(t),
\]

we obtain, (similarly as in Ref. [6])

\[
\Delta \tilde{\rho}_{AB}(t) = \left( \frac{1}{i\hbar} \right) \int_{t}^{t+\Delta t} dt_1 \left[ \tilde{V}_{AB}(t_1), \tilde{\rho}_{AB}(t) \right] + \left( \frac{1}{i\hbar} \right)^2 \int_{t}^{t+\Delta t} dt_1 \int_{t}^{t_1} dt_2 \left[ \tilde{V}_{AB}(t_1), \left[ \tilde{V}_{AB}(t_2), \tilde{\rho}_{AB}(t) \right] \right] + \left( \frac{1}{i\hbar} \right)^3 \int_{t}^{t+\Delta t} dt_1 \int_{t}^{t_1} dt_2 \int_{t}^{t_2} dt_3 \left[ \tilde{V}_{AB}(t_1), \left[ \tilde{V}_{AB}(t_2), \left[ \tilde{V}_{AB}(t_3), \tilde{\rho}_{AB}(t) \right] \right] \right].
\]

Higher order iterations will contain fourfold, etc., integrals and commutators. Let us note that in the last term we have time ordering \( t + \Delta t \geq t_1 \geq t_2 \geq t_3 \geq t \). The above equation is rigorous, no approximations have been made.

### 2.2 Weak-coupling approximation

Weak-coupling approximation (discussed in all Refs. [2]–[6]), consists in retaining the terms up to the second order in interaction hamiltonian. Higher order terms are then neglected. Thus, we remain with

\[
\Delta \tilde{\rho}_{AB}(t) = \left( \frac{1}{i\hbar} \right) \int_{t}^{t+\Delta t} dt_1 \left[ \tilde{V}_{AB}(t_1), \tilde{\rho}_{AB}(t) \right] + \left( \frac{1}{i\hbar} \right)^2 \int_{t}^{t+\Delta t} dt_1 \int_{t}^{t_1} dt_2 \left[ \tilde{V}_{AB}(t_1), \left[ \tilde{V}_{AB}(t_2), \tilde{\rho}_{AB}(t) \right] \right].
\]

Alternatively, we can say that the obtained equation is valid in the second-order perturbation theory. Such an approximation requires a justification. This will be presented in the Auxiliary sections, now we focus on further steps of the derivation.

Reduction of the operator \( \tilde{\rho}_{AB}(t) \) in the left hand side of (14) poses no difficulties. Tracing over the reservoir variables (subsystem \( \mathcal{B} \)) we obtain

\[
\Delta \tilde{\rho}_A(t) = \left( \frac{1}{i\hbar} \right) \int_{t}^{t+\Delta t} dt_1 \text{Tr}_B \left[ \tilde{V}_{AB}(t_1), \tilde{\rho}_{AB}(t) \right] + \left( \frac{1}{i\hbar} \right)^2 \int_{t}^{t+\Delta t} dt_1 \int_{t}^{t_1} dt_2 \text{Tr}_B \left[ \tilde{V}_{AB}(t_1), \left[ \tilde{V}_{AB}(t_2), \tilde{\rho}_{AB}(t) \right] \right].
\]
This expression has certain drawback. The the commutators in the right hand side
contain full density operator \( \tilde{\rho}_{AB}(t) \), and not the interesting (relevant) reduced one
\( \tilde{\rho}_A(t) \). To proceed, we need some more assumptions and approximations.

One more remark seems to be in place. Subsequent iterations leading to Eq. (13)
are rigorous. In equation (15) – which is approximate – there occurs the operator
\( \rho_{AB}(t) \), taken at the initial moment. The last term in the exact equation (13)
contains \( \tilde{\rho}_{AB} \) for moments earlier than the current moment \( t + \Delta t \), but later than
the initial instant \( t \). This means that we neglect the influence of the "history" on
the present moment. We shall return to the discussion of this point.

2.3 Neglecting the initial correlations

The key role in our consideration is played by the assumption that there are two
distinct time scales \([6]\). The first one is specified by \( \tau_B \) – typical time during which
the internal correlations in the reservoir \( B \) exist. This will discussed in more detail
later. Here we will only say that \( \tau_B \) is such a time, that when it elapses, the state
of the reservoir is practically independent of its initial state. The second scale is
provide by time \( T_A \). It characterizes the evolution (changes) of the operator \( \tilde{\rho}_A(t) \)
which is (are) due to the interaction with reservoir, and which may be specified by
the relation
\[
\frac{\Delta \tilde{\rho}_A(t)}{\Delta t} \sim \frac{1}{T_A} \tilde{\rho}_A(t). \tag{16}
\]

Time \( T_A \) may be called the characteristic relaxation time of subsystem \( A \). Let us
note that we are speaking about interaction – the interaction picture we employ is
thus, particularly useful. We make no statements about the rate of the free evolution
of \( \rho_A \) (in the Schrödinger picture), which is governed by hamilto nian \( H_A \). Usually,
the characteristic times of free evolution (the times of the order of \( \tau_A \sim \langle H_A \rangle_A / \hbar \))
are typically much shorter that \( T_A \) describing the influence of the interaction between
subsystems \([6]\).

Now, we assume that the introduced time scales satisfy the requirement
\[
\tau_B \ll \Delta t \ll T_A. \tag{17}
\]

We have a fast scale (small \( \tau_B \)) determining the decay of correlations within the
reservoir and the second – much slower – scale defined by relatively long relaxation
time \( T_A \), characterizing the interaction between the two parts of the entire physical
system. This may be phrased differently. We have assumed that the interaction is
weak. Let \( V \) denote the average ”strength” of this interaction. Uncertainty principle
states that
\[
VT_A \sim \hbar \quad \Rightarrow \quad T_A \sim \frac{\hbar}{V}. \tag{18}
\]

The condition \( \tau_B \ll T_A \) implies that
\[
\tau_B \ll T_A \sim \frac{\hbar}{V} \quad \Rightarrow \quad \frac{V \tau_B}{\hbar} \ll 1. \tag{19}
\]
In other words, we can say that spectral widths are the reciprocals of characteristic times, so the condition \( \tau_B \ll T_A \) means that the spectral width of the reservoir energies must be much larger than the spectral width of the interaction between subsystem \( \mathcal{A} \) with reservoir. Further discussion and justification of our approximations is postponed to Auxiliary sections. Here we focus on the derivation of the master equation.

The adopted assumption \( \tau_B \ll T_A \) allows us to make the approximation which is sometimes called the Born one [3]-[6]. Initial density operator for the whole system \( \mathcal{A} + \mathcal{B} \) can always be written as

\[
\bar{\rho}_{AB}(t) = \bar{\rho}_A(t) \otimes \bar{\rho}_B(t) + \bar{\rho}_{\text{corel}}(t),
\]

where \( \bar{\rho}_A(t) \) and \( \bar{\rho}_B(t) \) are the reduced density operators for two subsystems. The state of the whole system consists of a factorizable part \( \bar{\rho}_A(t) \otimes \bar{\rho}_B(t) \) and the entangled part \( \bar{\rho}_{\text{corel}}(t) \), describing the interaction-induced correlations between the subsystems. Equation (15) gives us the change \( \Delta \bar{\rho}_A(t) = \bar{\rho}_A(t+\Delta t) - \bar{\rho}_A(t) \), hence informs us about changes occurring in the time interval \( \Delta t \). Assumption that \( \tau_B \ll \Delta t \) allows us to neglect the mentioned correlations. As previously, we postpone the discussion for Auxiliary sections. At present, we assume that

\[
\bar{\rho}_{AB}(t) \approx \bar{\rho}_A(t) \otimes \bar{\rho}_B(t).
\]

By assumption, the reservoir (environment) is large, its correlation time is very short, so the reservoir’s relaxation is fast. We may say that before any significant changes occur in subsystem \( \mathcal{A} \), the reservoir would have enough time to reach thermodynamic equilibrium. As it is known from statistical physics such state is given as

\[
\bar{\sigma}_B = \sum_z p(z) | z \rangle \langle z |, \quad \text{where} \quad p(z) = \frac{1}{Z} \exp \left( -\frac{E_z}{k_B T} \right).
\]

The quantity \( Z \) is a partition sum

\[
Z = \sum_z \exp \left( -\frac{E_z}{k_B T} \right).
\]

States \( | z \rangle \) and energies \( E_z \) are the eigenstates and eigenvalues of the reservoir hamiltonian, which can be written as \( H_B = \sum_z E_z | z \rangle \langle z | \). As a consequence we conclude that

\[
[\bar{\sigma}_B, H_B] = 0,
\]

so we can say that operator \( \bar{\sigma}_B \) is stationary – does not change in time. It is worth noting that we could have reversed the argument. First require stationarity, as expressed by (24) which would entail relations (22) and (23). Moreover, commutation
relation (24) implies that the reduced density operator $\bar{\sigma}_B$ is of the same form both in Schrödinger and interaction pictures.

Due to these remarks operator $\tilde{\rho}_B(t)$ appearing in Eq.(21) is simply replaced by $\bar{\sigma}_B$. Therefore, in Eq.(15) we make the replacement $\tilde{\rho}_{AB} = \tilde{\rho}_A(t) \otimes \bar{\sigma}_B$. So, we now have

$$\Delta \tilde{\rho}_A(t) = \left(\frac{1}{i\hbar}\right)^t \int_t^{t+\Delta t} dt_1 \text{Tr}_B[\tilde{V}_{AB}(t_1), \tilde{\rho}_A(t) \otimes \bar{\sigma}_B]$$

$$+ \left(\frac{1}{i\hbar}\right)^2 \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \text{Tr}_B[\tilde{V}_{AB}(t_1), [\tilde{V}_{AB}(t_2), \tilde{\rho}_A(t) \otimes \bar{\sigma}_B]].$$

The employed simplification facilitates computation of the remaining traces. However, to proceed effectively, we need to specify the interaction hamiltonian.

3 Interaction hamiltonian and its properties

3.1 The form of $\tilde{V}_{AB}(t)$

Our next assumption concerns the shape of the interaction hamiltonian. It is taken as (similarly as in the given references)

$$V_{AB} = \sum_{\alpha} A_{\alpha} \otimes X_{\alpha} = \sum_{\alpha} A_{\alpha}^\dagger \otimes X_{\alpha}^\dagger,$$

where $A_{\alpha}$ are operators which act in the space of the states of subsystem $A$, while operators $X_{\alpha}$ correspond to space of the reservoir’s states. Operators appearing in the definition (26) need not be hermitian (each one separately). Only the hamiltonian $V_{AB}$ must be hermitian. That is why we have written the second equality. We can say that to each nonhermitian term $A_{\alpha} \otimes X_{\alpha}$ corresponds the term $A_{\alpha}^\dagger \otimes X_{\alpha}^\dagger$, and the latter appears in the sum $V_{AB}$, but with another number. In Auxilliary sections we will argue that it is not any limitation. It is only important that the whole hamiltonian $V_{AB}$ must be hermitian.

Operators $A_{\alpha}$ and $X_{\alpha}$ act in different spaces so they are independent and commute. In the interaction picture we immediately have

$$\tilde{V}_{AB}(t) = \sum_{\alpha} \tilde{A}_{\alpha}(t) \otimes \tilde{X}_{\alpha}(t) = \sum_{\alpha} \tilde{A}_{\alpha}^\dagger(t) \otimes \tilde{X}_{\alpha}^\dagger(t),$$

with

$$\tilde{A}_{\alpha}(t) = e^{iHA_{\alpha}/\hbar} A_{\alpha} e^{-iHA_{\alpha}/\hbar}, \quad \tilde{X}_{\alpha}(t) = e^{iHB_{\alpha}/\hbar} X_{\alpha} e^{-iHB_{\alpha}/\hbar}.$$
We now make one more assumption about reservoir. We have already taken \( \bar{\rho}_B(t) \approx \bar{\sigma}_B \). Here, we assume that in the Schrödinger picture

\[
\langle X_\alpha \rangle_B \approx \text{Tr}_B \{ X_\alpha \rho_B(t) \} = \text{Tr}_B \{ X_\alpha \bar{\sigma}_B \} = 0.
\]

(29)

This assumption easily transforms to interaction picture

\[
\langle \tilde{X}_\alpha(t) \rangle_B = \text{Tr}_B \left\{ e^{i H_B t / \hbar} X_\alpha e^{-i H_B t / \hbar} \bar{\sigma}_B \right\} = \text{Tr}_B \{ X_\alpha \bar{\sigma}_B \} = 0,
\]

(30)

which follows from commutation relation (24), cyclic property of trace and (29). This is rather a simplification, not a restrictive assumption. This will be clarified and explained in Auxiliary sections. Eq. (29) (leading to (30)) allows us to see that the first term in the ME (25) is, in fact, zero. Indeed

\[
\text{Tr}_B \left[ \tilde{V}_{AB}(t_1), \tilde{X}_\alpha(t_1) \right] \text{Tr}_B \left[ \tilde{V}_{AB}(t_2), \tilde{X}_\alpha(t_1) \right] = 0.
\]

(31)

Both traces are equal (cyclic property), nevertheless this expression need not be zero, because operators of the \( A \) system need not commute. If requirement (29) is not fulfilled then the above average may not vanish. Assumption (29) and its consequence (30) fortunately give zero, thus the first term of Eq. (25) vanishes and we remain with the master equation

\[
\Delta \tilde{\rho}_A(t) = \left( \frac{1}{i \hbar} \right)^2 \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \text{Tr}_B \left[ \tilde{V}_{AB}(t_1), \tilde{V}_{AB}(t_2), \tilde{\rho}_A(t) \otimes \bar{\sigma}_B \right].
\]

(32)

Expanding the commutators is simple. Moreover, one easily notices that there are two pairs of hermitian conjugates. Hence we have

\[
\frac{\Delta \tilde{\rho}_A(t)}{\Delta t} = \frac{1}{\hbar^2} \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \text{Tr}_B \left\{ \tilde{V}_{AB}(t_2) \left( \tilde{\rho}_A(t) \otimes \bar{\sigma}_B \right) \tilde{V}_{AB}(t_1) \right\} + \mathbb{H} \mathbb{C}.
\]

(33)

We can now use hamiltonian (27) and perform further transformations. It can be, however, shown \([2]–[4]\) that this equation does not guarantee that the positivity of the density operator \( \tilde{\rho}_A(t) \) is preserved. It appears that the so-called secular approximation is necessary. To perform it effectively, it is convenient to present the interaction hamiltonian in a somewhat different form.
3.2 Operators $A_\alpha(\Omega)$

Let us write the hamiltonian of the subsystem $A$ as

$$H_A = \sum_a \hbar \omega_a |a\rangle \langle a|.$$  \hspace{1cm} (34)

States $|a\rangle$ constitute the complete and orthonormal basis in the space of states of the subsystem $A$. The eigenfrequencies $\omega_a$ may or may not be degenerate. We allow $\omega_a = \omega_b$ for $a \neq b$. At present it suffices that we distinguish different kets $|a\rangle$ solely by their "quantum number" $a$. Similarly as in Refs.[3, 4], we now define the operators $A_\alpha(\Omega)$ via the following relation

$$A_\alpha(\Omega) = \sum_{a,b} \delta(\omega_{ba} - \Omega) |a\rangle \langle a| A_\alpha |b\rangle \langle b|.$$  \hspace{1cm} (35)

This representation may be called the decomposition of operator $A_\alpha$ into eigen-projectors of hamiltonian $H_A$. Delta $\delta(\omega_{ba} - \Omega)$ is of the Kronecker type, that is

$$\delta(\omega_{ba} - \Omega) = \begin{cases} 0 & \text{for } \omega_{ba} \neq \Omega, \\ 1 & \text{for } \omega_{ba} = \Omega, \end{cases}$$  \hspace{1cm} (36)

In our considerations we allow for nonhermitian operators $A_\alpha$. Hence, definition (35) is augmented by the following one

$$A_\alpha^\dagger(\Omega) = \sum_{a,b} \delta(\omega_{ab} - \Omega) |b\rangle \langle b| A_\alpha^\dagger |a\rangle \langle a|$$

$$= \sum_{a,b} \delta(\omega_{ab} - \Omega) |a\rangle \langle a| A_\alpha^\dagger |b\rangle \langle b|,$$  \hspace{1cm} (37)

because it is always allowed to interchange the summation indices $a \leftrightarrow b$. We stress that $A_\alpha(\Omega)$ contains Bohr frequency $\omega_{ba}$, while in $A_\alpha^\dagger(\Omega)$ we have $\omega_{ab} = -\omega_{ba}$. The following relation seems to be quite obvious

$$\sum_\Omega \delta(\omega_{kn} - \Omega) = 1,$$  \hspace{1cm} (38)

since out of all $\Omega$’s one will exactly match $\omega_{kn}$. As a consequence we obtain

$$\sum_\Omega A_\alpha(\Omega) = A_\alpha.$$  \hspace{1cm} (39)

Indeed, from definition (35), relation (38) and due to completeness of states $|a\rangle$ we get

$$\sum_\Omega A_\alpha(\Omega) = \sum_\Omega \sum_{a,b} \delta(\omega_{ba} - \Omega) |a\rangle \langle a| A_\alpha |b\rangle \langle b|$$

$$= \sum_{a,b} |a\rangle \langle a| A_\alpha |b\rangle \langle b| = 1A_\alpha 1 = A_\alpha.$$  \hspace{1cm} (40)
Relation (39) implies that the interaction hamiltonian (in Schrödinger picture) can be written as

\[ V_{AB} = \sum_{\alpha} A_{\alpha} \otimes X_{\alpha} = \sum_{\Omega} \sum_{\alpha} A_{\alpha}(\Omega) \otimes X_{\alpha}. \]  

(41)

Similarly as above we can also show that

\[ \sum_{\Omega} A_{\alpha}^\dagger(\Omega) = A_{\alpha}^\dagger, \]  

(42)

and

\[ V_{AB} = V_{AB}^\dagger = \sum_{\Omega} \sum_{\alpha} A_{\alpha}^\dagger(\Omega) \otimes X_{\alpha}^\dagger. \]  

(43)

Using definition (35) we find the operator \( \widetilde{A}_j(\Omega) \) in the interaction picture

\[ \widetilde{A}_\alpha(\Omega) = e^{iH_A t/\hbar} A_{\alpha}(\Omega) \left. e^{-iH_A t/\hbar} \right| a \rangle = e^{i\omega_a t} \left| a \right\rangle. \]  

(44)

Because \( e^{iH_A t/\hbar} \left| a \right\rangle = e^{i\omega_a t} \left| a \right\rangle \). Linking expressions (41) and (44) we write the interaction hamiltonian in the interaction picture

\[ \widetilde{V}_{AB}(t) = \sum_{\Omega} \sum_{\alpha} e^{-i\Omega t} A_{\alpha}(\Omega) \otimes \tilde{X}_{\alpha}^\dagger(t) = \sum_{\Omega} \sum_{\alpha} e^{i\Omega t} A_{\alpha}^\dagger(\Omega) \otimes \tilde{X}_{\alpha}^\dagger(t) = \widetilde{V}_{AB}(t). \]  

(45)

Before starting to analyze ME (33), let us notice that operators \( A_{\alpha}(\Omega) \) possess some interesting properties [3]. Discussion of these properties is moved to Auxiliary sections.

### 3.3 Further analysis of master equation

We return to master equation (33). Interaction hamiltonian \( \widetilde{V}_{AB}(t_2) \) is taken as in the first part of Eq. (45), while \( \widetilde{V}_{AB}(t_1) \) is represented by its hermitian conjugate according to second part of (45). This gives

\[
\frac{\Delta \tilde{Q}_A(t)}{\Delta t} = \frac{1}{\hbar^2} \sum_{\alpha, \beta, \Omega, \Omega'} \int_t^{t+\Delta t} dt_1 \int_t^{t+\Delta t} dt_2 \sum_{\alpha, \beta} \sum_{\Omega, \Omega'} \mathrm{Tr}_B \left\{ e^{-i\Omega t_2} A_{\beta}(\Omega) \otimes \tilde{X}_{\beta}(t_2) \left[ \tilde{q}_A(t) \otimes \tilde{\sigma}_B \right] e^{i\Omega' t_1} A_{\alpha}^\dagger(\Omega') \otimes \tilde{X}_{\alpha}^\dagger(t_1) \right. \\
\left. - e^{i\Omega' t_1} A_{\alpha}^\dagger(\Omega') \otimes \tilde{X}_{\alpha}^\dagger(t_1) \left[ e^{-i\Omega t_2} A_{\beta}(\Omega) \otimes \tilde{X}_{\beta}(t_2) \right] \tilde{q}_A(t) \otimes \tilde{\sigma}_B \right\} + \mathrm{H.C.}
\]  

(46)

Computing tensor products we remember that partial trace is taken only with respect to reservoir variables. Moreover, we note that these traces are the same (cyclic property). Therefore we denote

\[ \tilde{G}_{\alpha\beta}(t_1 - t_2) = \mathrm{Tr}_B \left\{ \tilde{X}_{\alpha}^\dagger(t_1) \tilde{X}_{\beta}(t_2) \tilde{\sigma}_B \right\}. \]  

(47)
Finally we rewrite the arguments of the exponentials as \( i\Omega' t_1 - i\Omega t_2 = i(\Omega' - \Omega)t_1 + i\Omega(t_1 - t_2) \). Thus Eq.\((46)\) becomes

\[
\frac{\Delta \bar{g}_A(t)}{\Delta t} = \frac{1}{\hbar^2} \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \sum_{\alpha,\beta} \sum_{\Omega,\Omega'} e^{i(\Omega' - \Omega)t_1} e^{i\Omega(t_1 - t_2)} \bar{G}_{\alpha\beta}(t_1 - t_2)
\]

\[
\times \left[ A_\beta(\Omega)\bar{g}_A(t)A^\dagger_\alpha(\Omega') - A^\dagger_\alpha(\Omega')A_\beta(\Omega)\bar{g}_A(t) \right] + \mathbb{H.C.} \quad (48)
\]

The quantity \( \bar{G}_{\alpha\beta}(t_1 - t_2) \) is called the correlation function of the reservoir. We will briefly discuss its properties.

### 3.4 Correlation functions \( \bar{G}_{\alpha\beta} \)

Let us focus on the functions defined by the right hand side of Eq.\((47)\), that is

\[
G_{\alpha\beta}(t_1, t_2) = \text{Tr}_B \left\{ \bar{X}_\alpha(t_1) \bar{X}_\beta(t_2) \bar{\sigma}_B \right\} \quad (49)
\]

These are the functions of two variables and it is not, a priori, clear that they depend only of the difference \( \tau = t_1 - t_2 \). Before discussing this fact, let us note that \( G^*_{\alpha\beta}(t_1, t_2) = G_{\beta\alpha}(t_2, t_1) \). To prove this relation, we recall that \( \text{Tr}_B \{ A \} = \text{Tr}_B \{ A^\dagger \} \), so that the definition \((49)\) gives

\[
G^*_{\alpha\beta}(t_1, t_2) = \text{Tr}_B \left\{ \bar{\sigma}_B \bar{X}_\beta(t_2) \bar{X}_\alpha(t_1) \right\}
\]

\[
= \text{Tr}_B \left\{ \bar{X}_\beta(t_2) \bar{X}_\alpha(t_1) \bar{\sigma}_B \right\} = G_{\beta\alpha}(t_2, t_1) \quad (50)
\]

Now, we will show that the function \( G_{\alpha\beta}(t_1, t_2) \) is indeed a function of the difference of its arguments. The key role plays the fact that the state of the reservoir (density operator \( \bar{\sigma}_B \)) is stationary (does not change in time). Explicitly using the interaction picture we get

\[
G_{\alpha\beta}(t_1, t_2) = \text{Tr}_B \left\{ (e^{iH_B t_1}/\hbar) X^\dagger_\alpha e^{-iH_B t_1}/\hbar) (e^{iH_B t_2}/\hbar) X_\beta e^{-iH_B t_2}/\hbar) \bar{\sigma}_B \right\} \quad (51)
\]

The trace is cyclic and \( \bar{\sigma}_B \) commutes with hamiltonian \( H_B \) so we conclude that

\[
G_{\alpha\beta}(t_1, t_2) = \text{Tr}_B \left\{ e^{iH_B (t_1 - t_2)/\hbar} X^\dagger_\alpha e^{-iH_B (t_1 - t_2)/\hbar} X_\beta \bar{\sigma}_B \right\}
\]

\[
= \text{Tr}_B \left\{ \bar{X}_\alpha^\dagger(t_1 - t_2) \bar{X}_\beta(0) \bar{\sigma}_B \right\} = \bar{G}_{\alpha\beta}(\tau = t_1 - t_2) \quad (52)
\]

for two moments of time \( t_1 > t_2 \). Reservoir’s correlation function effectively depends only on one variable. This fact is denoted by a bar over the symbol of correlation function. Thus we write

\[
G_{\alpha\beta}(t_1, t_2) = \bar{G}_{\alpha\beta}(\tau) = \text{Tr}_B \left\{ \bar{X}_\alpha^\dagger(\tau) X_\beta \bar{\sigma}_B \right\} \quad (53)
\]
Such correlation functions are called stationary. Sometimes the concept of stationarity means invariance with respect to time translation. Indeed, for arbitrary time $T$ we have

$$\bar{G}_{\alpha\beta}(t_1 + T, t_2 + T) = \bar{G}_{\alpha\beta}\left((t_1 + T) - (t_2 + T)\right) = \bar{G}_{\alpha\beta}(t_1 - t_2).$$ (54)

This property of the correlation functions is a straightforward consequence of the stationarity of reservoir’s density operator $\bar{\sigma}_B$.

4 Discussion of times

Preparing this section of our tutorial we greatly benefited from the analogous discussion by Cohen-Tannoudji et al. To large extent we follow their reasoning, trying to elucidate some less obvious points. Admitting this, we will refrain from giving multiple references to their work.

4.1 Limits of the integrals and Markov approximation

In master equation (48) one integrates over the triangle $ABC$ which is shown in Fig. 1. Firstly, one computes the integral over $dt_2$ in the range from $t$ to $t_1$. This is indicated by thin vertical lines (at left). Next, one sums such contributions by integrating over $dt_1$ from $t$ to $t + \Delta t$. The integrand in (48) contains correlation functions of the reservoir which depend on the difference $\tau = t_1 - t_2$. We stress that we always have $t_1 \geq t_2$, so that $\tau \geq 0$. The integration over the triangle can be performed in another manner.

Let us consider the geometry (right graph in Fig. 1). Along the diagonal AC we have $t_1 = t_2$, so $\tau = t_1 - t_2 = 0$. The straight line $l_1$ has (in $t_1$ and $t_2$ variables) the

Figure 1: Left figure presents the integration region in the double integral in Eq. (48). Right figure illustrates the change to new variables $\tau = t_1 - t_2$ and $t_1$. Other explanations are to be found in the text.
equation \( t_2 = t_1 - \tau \), where \( \tau \) is fixed, since \((-\tau)\) is the coordinate \( t_2 \) of the point where the discussed line intersects the axis \( t_2 \). Then, for the line \( l_k \) (passing through point B) \( \tau \) is also fixed (by the same argument, as in the case of line \( l_1 \)). On \( l_k \), at the point B we have \( t_1 = t + \Delta t \) and \( t_2 = t \). Thus, we have \( \tau = \Delta t \). Parameter \( \tau \) specifies the skew straight lines (parallel to the diagonal AC) and passing through triangle ABC. Integration over the triangle ABC is now done as follows. We fix \( \tau \in (0, \Delta t) \) and we move along the segment \( A'C' \) (see Fig.2). Variable \( t_1 \) runs in the interval from \( t + \tau \) to \( t + \Delta t \). So, we first integrate over \( dt_1 \) from \( t + \tau \) to \( t + \Delta t \) (along the segment \( A'C' \)). Next, we integrate over \( d\tau \) from zero to \( \Delta t \). In this manner we sum the contributions from all skew segments covering the triangle ABC. Therefore, we can write

\[
\int_{t}^{t+\Delta t} dt_1 \int_{t}^{t_1} dt_2 = \int_{0}^{\Delta t} d\tau \int_{t+\tau}^{t+\Delta t} dt_1,
\]

while we remember that \( \tau = t_1 - t_2 \) (or \( t_2 = t_1 - \tau \)). Performing the discussed changes of integration variables in Eq. (48), we get

\[
\Delta \tilde{g}_A(t) = \frac{1}{\hbar^2 \Delta t} \int_{0}^{\Delta t} d\tau \int_{t+\tau}^{t+\Delta t} dt_1 \sum_{\alpha,\beta} \sum_{\Omega,\Omega'} e^{i(\Omega'-\Omega)t_1} e^{i\Omega\tau} \tilde{C}_{\alpha\beta}(\tau) \\
\times \left[ A_\beta(\Omega) \tilde{g}_A(t) A_\alpha^\dagger(\Omega') - A_\alpha^\dagger(\Omega') A_\beta(\Omega) \tilde{g}_A(t) \right] + \mathbb{H.C.},
\]

We recall that the considered time intervals satisfy the requirement \( \Delta t \gg \tau_B \) (which will be discussed in detail later). If it is true, then the main contribution to the integral over \( d\tau \) in Eq. (56) will come from the region in the neighborhood of \( 0 \leq \tau \leq \Delta t \).
\[ \tau < \tau_B \ll \Delta t. \] Geometrically, this corresponds to a narrow belt which is parallel to the diagonal AC and lies just below it. It follows, that outside this region the reservoir’s correlation functions practically vanish (decay to zero). Therefore, we will not make any serious error moving the upper limit of integration over \( d\tau \) to infinity. Moreover, since only small \( \tau \)’s contribute significantly, the lower limit of the integral over \( dt_1 \) may be approximated simply by \( t \), so only a small "initial" error might be introduced. With these approximations equation (56) yields

\[
\frac{\Delta \tilde{\rho}_A(t)}{\Delta t} = \frac{1}{\hbar^2 \Delta t} \sum_{\Omega,\Omega',\alpha,\beta} \int_0^\infty d\tau e^{i\Omega\tau} \bar{G}_{\alpha\beta}(\tau) \int_t^{t+\Delta t} dt_1 e^{i(\Omega' - \Omega)t_1} \times \left[ A_\beta(\Omega)\tilde{g}_A(t)A_\alpha(\Omega') - A_\alpha(\Omega')A_\beta(\Omega)\tilde{g}_A(t) \right] + \mathbb{H.C.} \tag{57}
\]

Introducing the quantities

\[
J(\Omega' - \Omega) = \frac{1}{\Delta t} \int_t^{t+\Delta t} dt_1 \exp\left[ i(\Omega' - \Omega)t_1 \right], \tag{58a}
\]

\[
W_{\alpha\beta}(\Omega) = \int_0^\infty d\tau e^{i\Omega\tau} \bar{G}_{\alpha\beta}(\tau) = \int_0^\infty d\tau e^{i\Omega\tau} \text{Tr}_B\{\tilde{X}_\alpha^\dagger(\tau) X_\beta \sigma_B\}, \tag{58b}
\]

we rewrite Eq. (57) as follows

\[
\frac{\Delta \tilde{\rho}_A(t)}{\Delta t} = \frac{1}{\hbar^2 \Delta t} \sum_{\Omega,\Omega',\alpha,\beta} J(\Omega' - \Omega)W_{\alpha\beta}(\Omega) \times \left[ A_\beta(\Omega)\tilde{g}_A(t)A_\alpha(\Omega') - A_\alpha(\Omega')A_\beta(\Omega)\tilde{g}_A(t) \right] + \mathbb{H.C.} \tag{59}
\]

This equation specifies the rate of change of the reduced density operator \( \tilde{g}_A(t) \) within the time interval \((t, t + \Delta t)\). The quotient \( \Delta \tilde{\rho}_A(t) / \Delta t \) can be treated as an averaging

\[
\frac{\Delta \tilde{\rho}_A(t)}{\Delta t} = \frac{\tilde{\rho}_A(t + \Delta t) - \tilde{\rho}_A(t)}{\Delta t} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \frac{d\tilde{\rho}_A(t)}{dt} dt_1. \tag{60}
\]

This averaging results in smoothing all very rapid changes of \( \tilde{\rho}_A(t) \) which may occur during the interval \((t, t + \Delta t)\). In principle we should account for such rapid changes. We do not do that because right hand side of Eq. (59) contains \( \tilde{\rho}_A(t) \), while the left hand side represents the smoothed rate of change. This rate depends on the density operator \( \tilde{\rho}_A \) in the past, that is at the moment when the smoothed evolution was started. So our next approximation consists in replacing the smoothed rate by a usual derivative. In other words, the variation at an instant \( t \) (that is the derivative \( d\tilde{\rho}_A(t)/dt \)) is connected with the value of \( \tilde{\rho}_A(t) \) at the very same instant. This approximation allows us to use a usual derivative at the left hand side of (59). This approximation sometimes is called a Markovian one since it connects the variations...
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of some physical quantity with its value at the same instant, independently from
the values which this quantity had at earlier moments. We can say that Markovian
approximation consists in neglecting the influence of the history of the physical
system on its current state which fully determines the presently occurring changes.
In some literature sources this approximation is also called the coarse-graining one,
because small and rapid fluctuations are neglected when the evolution is investigated
on a much longer time scale specified by $\Delta t$.

With all the discussed approximation our master equation (59) becomes

$$\frac{d}{dt} \tilde{\varrho}_A(t) = \frac{1}{\hbar} \sum_{\Omega, \Omega', \alpha, \beta} J(\Omega' - \Omega) W_{\alpha \beta}(\Omega)
\times \left[ A_\beta(\Omega) \tilde{\varrho}_A(t) A_\alpha^\dagger(\Omega') - A_\alpha^\dagger(\Omega') A_\beta(\Omega) \tilde{\varrho}_A(t) \right] + \mathbb{H.C.} \quad (61)$$

4.2 Schrödinger picture

At this stage, we return to the Schrödinger picture and we insert

$$\tilde{\varrho}_A(t) = e^{iH_A t/\hbar} \rho_A(t) e^{-iH_A t/\hbar}, \quad (62)$$

into Eq. (61). When computing the derivative at the left hand side we reproduce
the free evolution term. Thus, from (61) we get

$$e^{iH_A t/\hbar} \left( \frac{d}{dt} \rho_A(t) \right) e^{-iH_A t/\hbar} = -\frac{i}{\hbar} e^{iH_A t/\hbar} \left[ H_A, \rho_A(t) \right] e^{-iH_A t/\hbar}
+ \left\{ \frac{1}{\hbar^2} \sum_{\Omega, \Omega', \alpha, \beta} J(\Omega' - \Omega) W_{\alpha \beta}(\Omega)
\times \left[ A_\beta(\Omega) e^{iH_A t/\hbar} \rho_A(t) e^{-iH_A t/\hbar} A_\alpha^\dagger(\Omega')
- A_\alpha^\dagger(\Omega') A_\beta(\Omega) e^{iH_A t/\hbar} \rho_A(t) e^{-iH_A t/\hbar} \right] + \mathbb{H.C.} \right\}. \quad (63)$$

Multiplying on the left by $e^{-iH_A t/\hbar}$ and on the right by $e^{iH_A t/\hbar}$, we use relation (44)
and its hermitian conjugate (for negative times). This yields

$$\frac{d}{dt} \rho_A(t) = -\frac{i}{\hbar} \left[ H_A, \rho_A(t) \right] + \left\{ \frac{1}{\hbar^2} \sum_{\Omega, \Omega', \alpha, \beta} J(\Omega' - \Omega) W_{\alpha \beta}(\Omega) e^{i(\Omega - \Omega') t}
\times \left[ A_\beta(\Omega) \rho_A(t) A_\alpha^\dagger(\Omega') - A_\alpha^\dagger(\Omega') A_\beta(\Omega) \rho_A(t) \right] + \mathbb{H.C.} \right\}. \quad (64)$$

4.3 Integral $J(\Omega' - \Omega)$ and secular approximation

Our master equation contains the integral $J(\Omega' - \Omega)$ defined in (58a). Its computation
is straightforward. Denoting temporarily $x = \Omega' - \Omega$, we get

$$J(x) = \int_t^{t+\Delta t} dt_1 \frac{e^{ixt_1}}{\Delta t} = e^{ixt+x\Delta t/2} \frac{\sin \left( \frac{x\Delta t}{2} \right)}{\frac{x\Delta t}{2}} = e^{ixt} F(x), \quad (65)$$

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where we have introduced (as in [6]) a function specified as

\[ F(x) = e^{ix\Delta t/2} \frac{\sin \left( \frac{x\Delta t}{2} \right)}{\left( \frac{x\Delta t}{2} \right)}. \] (66)

Due to the obtained results we can write

\[ J(\Omega' - \Omega) = e^{i(\Omega' - \Omega)t} F(\Omega' - \Omega). \] (67)

Inserting the computed integral into (64) we note that the exponential factor cancels out. Hence

\[
\frac{d}{dt} \rho_A(t) = -\frac{i}{\hbar} \left[ H_A, \rho_A(t) \right] + \left\{ \frac{1}{\hbar^2} \sum_{\Omega',\Omega} \sum_{\alpha,\beta} F(\Omega' - \Omega) W_{\alpha\beta}(\Omega) \times \left[ A_{\beta}(\Omega) \rho_A(t) A_\alpha^\dagger(\Omega) - A_\alpha^\dagger(\Omega) A_{\beta}(\Omega) \rho_A(t) \right] + \mathbb{H.C} \right\}. \] (68)

The sense of function \( F(\Omega' - \Omega) \) must be carefully considered. We proceed along the lines similar to those in [6]. It is easy to see that function \( |F(x)| \) has a sharp maximum for \( x = \Omega' - \Omega = 0 \), where it is equal to unity.

![Figure 3: The graph of the modulus of the function \( F(\Omega' - \Omega) \) which appears in (68). If the time \( \Delta t \) is sufficiently large then the graph has a sharp maximum for \( \Omega' = \Omega \).](image)

Zeroes of this function correspond to

\[
\frac{1}{2}x\Delta t = n\pi \quad \implies \quad x = \frac{2n\pi}{\Delta t}. \] (69)

If the time \( \Delta t \) is sufficiently long then the central maximum is very narrow. The question is what does it mean "sufficiently long time". Let us consider two possibilities.

1. If \( x = |\Omega' - \Omega| \ll (\Delta t)^{-1} \), the argument of function \( |F(x)| \) is very close to zero, its value being practically one.
2. If \( x = |\Omega' - \Omega| \gg (\Delta t)^{-1} \) (Bohr frequencies are significantly different) then \( |F(x)| \) is close to zero, as it is seen in Fig 3.

We conclude that the terms at the right hand side of master equation (68) containing the operator products \( A_\alpha^\dagger(\Omega') A_\beta(\Omega) \), for which \( |\Omega' - \Omega| \gg (\Delta t)^{-1} \) practically do not contribute to the evolution of the density operator \( \rho_A(t) \). According to the first possibility above, significant contributions come only from such couplings that operators \( A_\alpha^\dagger(\Omega') \) and \( A_\beta(\Omega) \) have practically equal Bohr frequencies.

As we know, time \( T_A \) is a characteristic relaxation time in subsystem \( A \) due to interaction with reservoir and it satisfies the estimate \( \Delta t \ll T_A \) (we discuss it later).

It can be argued (see also [6]) that the terms in master equation (68), in which \( |\Omega' - \Omega| \sim (\Delta t)^{-1} \) also give very small contributions, so that they can be neglected.

As a result of all these approximations, we may say that only those terms in right hand side of master equation (68) contribute significantly for which \( |\Omega' - \Omega| = 0 \). Such an approximation is called the secular one. It allows us to replace the function \( F(\Omega' - \Omega) \) by the Kronecker delta \( \delta(\Omega' - \Omega) \) defined as in (36). It reminds us that only the terms satisfying the requirement \( (\Omega' = \Omega) \) give nonzero contribution. All these arguments lead to master equation of the form

\[
\frac{d}{dt} \rho_A(t) = -\frac{i}{\hbar} \left[ H_A, \rho_A(t) \right] + \left\{ \frac{1}{\hbar^2} \sum_{\alpha,\beta} \sum_{\Omega'} \delta(\Omega' - \Omega) W_{\alpha\beta}(\Omega) \right.
\]
\[
\times \left[ A_\beta(\Omega) \rho_A(t) A_\alpha^\dagger(\Omega') - A_\alpha^\dagger(\Omega') A_\beta(\Omega) \rho_A(t) \right] + \mathbb{H.C.} \right\}. \tag{70}
\]

The presence of the discussed Kronecker delta simplifies one of the summations, which gives

\[
\frac{d}{dt} \rho_A(t) = -\frac{i}{\hbar} \left[ H_A, \rho_A(t) \right] + \left\{ \frac{1}{\hbar^2} \sum_{\alpha,\beta} \sum_{\Omega} W_{\alpha\beta}(\Omega) \left[ A_\beta(\Omega) \rho_A(t) A_\alpha^\dagger(\Omega) \right. \right.
\]
\[
\left. - A_\alpha^\dagger(\Omega) A_\beta(\Omega) \rho_A(t) \right] + \mathbb{H.C.} \right\}. \tag{71}
\]

The fundamental part of the microscopic derivation of the master equation is finished. We shall perform some transformations which have important, but rather cosmetic character. We want to transform master equation into the so-called standard form. All other comments are, as mentioned many times, left to Auxiliary sections.

5 Standard form

5.1 Introduction

Standard form is important, because it can be shown (see [2, 3, 4]) that this form guarantees preservation of hermiticity, normalization and, first of all, the positivity of the reduced density operator \( \rho_A \). If our master equation (71) can be brought
into the standard form, then we can be sure that all the necessary properties of the density operator of subsystem $A$ are indeed preserved. Obviously, the first term in the right hand side of equation (71) describes the unitary evolution, hence we shall concentrate only on the second term. Writing explicitly the hermitian conjugates, we have

$$
\frac{d}{dt} \rho_A(t) = \frac{1}{\hbar^2} \sum_{\alpha,\beta} W_{\alpha\beta}(\Omega) \left[ A_{\beta}(\Omega) \rho_A(t) A_{\alpha}^\dagger(\Omega) - A_{\alpha}^\dagger(\Omega) A_{\beta}(\Omega) \rho_A(t) \right]
\quad + \frac{1}{\hbar^2} \sum_{\alpha,\beta} W^*_{\alpha\beta}(\Omega) \left[ A_{\beta}(\Omega) A_{\alpha}^\dagger(\Omega) - A_{\alpha}^\dagger(\Omega) A_{\beta}(\Omega) \rho_A(t) \right],
$$

(72)

because operator $\rho_A(t)$ is hermitian (the proof that hermiticity is preserved will be presented in Auxiliary sections). In the second term we interchange the summation indices $\alpha \leftrightarrow \beta$ which gives

$$
\frac{d}{dt} \rho_A(t) = \frac{1}{\hbar^2} \sum_{\alpha,\beta} W_{\alpha\beta}(\Omega) \left[ A_{\beta}(\Omega) \rho_A(t) A_{\alpha}^\dagger(\Omega) - A_{\alpha}^\dagger(\Omega) A_{\beta}(\Omega) \rho_A(t) \right]
\quad + \frac{1}{\hbar^2} \sum_{\alpha,\beta} W^*_{\alpha\beta}(\Omega) \left[ A_{\beta}(\Omega) A_{\alpha}^\dagger(\Omega) - A_{\alpha}^\dagger(\Omega) A_{\beta}(\Omega) \rho_A(t) \right].
$$

(73)

5.2 New notation

For further convenience we introduce the following notation

$$
\Gamma_{\alpha\beta}(\Omega) = W_{\alpha\beta}(\Omega) + W^*_{\beta\alpha}(\Omega),
$$

(74a)

$$
\Delta_{\alpha\beta}(\Omega) = \frac{1}{2i} \left[ W_{\alpha\beta}(\Omega) - W^*_{\beta\alpha}(\Omega) \right].
$$

(74b)

The matrix $\Gamma_{\alpha\beta}(\Omega)$ is hermitian and positively defined. The latter property is difficult to prove. It requires some advanced mathematics and we take this fact for granted. The readers are referred to literature [2, 3]. Hermiticity of $\Gamma_{\alpha\beta}$ follows directly from the definition (74a). Indeed, we have

$$
\Gamma^*_{\alpha\beta}(\Omega) = W^*_{\alpha\beta}(\Omega) + W^*_{\beta\alpha}(\Omega) = \Gamma_{\beta\alpha}(\Omega).
$$

(75)

The second matrix $\Delta_{\alpha\beta}(\Omega)$ is also hermitian. From (74b) it follows that

$$
\Delta^*_{\alpha\beta}(\Omega) = -\frac{1}{2i} \left[ W^*_{\alpha\beta}(\Omega) - W^*_{\beta\alpha}(\Omega) \right] = \frac{1}{2i} \left[ W_{\beta\alpha}(\Omega) - W^*_{\alpha\beta}(\Omega) \right] = \Delta_{\beta\alpha}(\Omega).
$$

(76)

Let us focus on the method of computation of elements $\Gamma_{\alpha\beta}(\Omega)$. As it will be shown, elements $\Delta_{\alpha\beta}(\Omega)$ are less important. To find $\Gamma_{\alpha\beta}$ we need quantities $W^*_{\beta\alpha}$. 

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Conjugating definition (58b) we find that
\[
W^*_{\beta\alpha}(\Omega) = \left( \int_0^\infty d\tau e^{i\Omega\tau} \text{Tr}_B \{ \tilde{X}_\beta^\dagger(\tau)X_\alpha\bar{\sigma}_B \} \right)^* = \int_0^\infty d\tau e^{-i\Omega\tau} \text{Tr}_B \{ X_\alpha\tilde{X}_\beta(\tau)\bar{\sigma}_B \} = \int_0^\infty d\tau e^{-i\Omega\tau} \text{Tr}_B \{ e^{-iH_B\tau/h}X_\alpha^\dagger e^{iH_B\tau/h}X_\beta\bar{\sigma}_B \},
\]
where we used relations (24), (28) and cyclic property of trace. Changing the integration variable \( \tau \to -\tau \), we have
\[
W^*_{\beta\alpha}(\Omega) = \int_{-\infty}^0 d\tau e^{i\Omega\tau} \text{Tr}_B \{ \tilde{X}_\alpha^\dagger(\tau)X_\beta\bar{\sigma}_B \}.
\]
(78)
The integrand is identical as in the definition (58b), only the integration limits are different. Combining this with (58b), we get
\[
\Gamma_{\alpha\beta}(\Omega) = \int_{-\infty}^\infty d\tau e^{i\Omega\tau} \text{Tr}_B \{ \tilde{X}_\alpha^\dagger(\tau)X_\beta\bar{\sigma}_B \} = \int_{-\infty}^\infty d\tau e^{i\Omega\tau} \tilde{G}_{\alpha\beta}(\tau).
\]
(79)
The elements \( \Gamma_{\alpha\beta}(\Omega) \) are the Fourier transforms of the corresponding correlation function of the reservoir.

Matrix \( \Delta_{\alpha\beta}(\Omega) \) does not have such a simple representation. From the definition (74b) and the second relation in (77)
\[
\Delta_{\alpha\beta}(\Omega) = \frac{1}{2i} \left[ \int_0^\infty d\tau e^{i\Omega\tau} \text{Tr}_B \{ \tilde{X}_\alpha^\dagger(\tau)X_\beta\bar{\sigma}_B \} - \int_0^\infty d\tau e^{-i\Omega\tau} \text{Tr}_B \{ X_\alpha\tilde{X}_\beta(\tau)\bar{\sigma}_B \} \right].
\]
(80)

5.3 Standard form

Inverting relations (74) we express elements \( W_{\alpha\beta} \) via \( \Gamma_{\alpha\beta} \) and \( \Delta_{\alpha\beta} \). After simple regrouping of the terms in Eq. (73) we find
\[
\frac{d}{dt} \rho_A(t) |_{\lambda} = \frac{1}{\hbar^2} \sum_{\Omega} \sum_{\alpha,\beta} \Gamma_{\alpha\beta}(\Omega) \left\{ A_\beta(\Omega) \rho_A(t) A_\alpha^\dagger(\Omega) - \frac{1}{2} \left[ A_\alpha^\dagger(\Omega) A_\beta(\Omega), \rho_A(t) \right]_+ - i\Delta_{\alpha\beta}(\Omega) \left[ A_\alpha^\dagger(\Omega)A_\beta(\Omega), \rho_A(t) \right] \right\}.
\]
(81)
Let us note that the last term is a commutator, so we define
\[
H_{LS} = \frac{1}{\hbar} \sum_{\Omega} \sum_{\alpha,\beta} \Delta_{\alpha\beta}(\Omega)A_\alpha^\dagger(\Omega)A_\beta(\Omega).
\]
(82)
Taking into account hermiticity of matrix \( \Delta_{\alpha\beta}(\omega) \) (changing the names of the summation indices when necessary) we can easily show that the operator \( H_{LS} \) is also
hermitian. Returning to full master equation, that is to Eq. (71), we conclude that the term containing $H_{LS}$ in (81) can be connected with the free hamiltonian one. In this manner, we finally have

$$\frac{d}{dt} \rho_A(t) = -\frac{i}{\hbar}[H_A + H_{LS}, \rho_A(t)]$$

$$+ \frac{1}{\hbar^2} \sum_{\Omega} \sum_{\alpha, \beta} \Delta_{\alpha \beta}(\Omega) \left\{ A_{\beta}(\Omega) \rho_A(t) A_{\alpha}^\dagger(\Omega) - \frac{1}{2} [A_{\alpha}^\dagger(\Omega) A_{\beta}(\Omega), \rho_A(t)]_+ \right\},$$

which coincides exactly with the standard form of the evolution equation for the reduced density operator $\rho_A(t)$ which describes the state of the subsystem $A$ interacting with reservoir $B$. This allows us to be sure that hermicity, normalization and positivity of the operator $\rho_A(t)$ are indeed ensured. Finally, let us remark that operator $H_{LS}$ which gives a contribution to the hamiltonian (unitary) evolution, usually produces small shifts of the eigenenergies of the subsystem $A$. That is why, in many practical applications, this term is simply omitted. This explains our previous remark that matrix $\Delta_{\alpha \beta}$ is less important than $\Gamma_{\alpha \beta}$. Obviously one can construct operator $H_{LS}$ and investigate its influence on the unperturbed energy levels of the subsystem $A$. Small energy shifts of eigenenergies of subsystem $A$ are qualitatively similar to the well-known Lamb shifts, which clarifies the employed notation.

The obtained master equation (83) is an operator one. In practice, we frequently need an equation of motion for the matrix elements of the reduced density operator $\rho_A(t)$. It seems to be natural to use the energy representation, that is to consider matrix elements of $\rho_A(t)$ calculated in the basis $\{|a\rangle\}$ of the eigenstates of the free hamiltonian $H_A$ (see Eq. (34)). This will be done in the next section.

5.4 Energy representation

When analyzing master equation in the basis of the eigenstates of free hamiltonian we need to be careful. The reason is that the commutator in (83) contains an additional term, namely the Lamb-shift hamiltonian. One may argue that this changes the hamiltonian and a new basis should be found (a basis in which $H_A + H_{LS}$ is diagonal). We will, however, proceed in the spirit of the perturbative approach. We will treat $H_{LS}$ as a small perturbation which, at most, will yield small energy shifts. Therefore, the set $\{|a\rangle\}$ of eigenstates of the unperturbed hamiltonian $H_A$ can be used as complete and orthonormal basis. Working within this scheme, we can easily construct master equation (equation of motion) for matrix elements of the density operator for subsystem $A$. We will suppress the index $A$ since it should lead to no misunderstanding. Taking matrix elements $\rho_{ab}(t) = \langle a | \rho_A(t) | b \rangle$ and
expanding the anticommutator term we obtain
\[
\frac{d}{dt} \rho_{ab}(t) = -\frac{i}{\hbar} \langle a \left| [H_A + H_{LS}, \rho(t)] \right| b \rangle \\
+ \frac{1}{\hbar^2} \sum_{\Omega, \alpha, \beta} \Gamma_{\alpha\beta}(\Omega) \left\{ \langle a \left| A_\beta(\Omega) \rho(t) A_\alpha^\dagger(\Omega) \right| b \rangle \right. \\
- \frac{1}{2} \langle a \left| A_\alpha^\dagger(\Omega) A_\beta(\Omega) \rho(t) \right| b \rangle - \frac{1}{2} \langle a \left| \rho(t) A_\alpha^\dagger(\Omega) A_\beta(\Omega) \right| b \rangle \right\}. \tag{84}
\]

The last three terms constitute a so-called dissipative term (or dissipator) and we will concentrate on its form. First, we use expressions (35), (37) for operators \( A_\alpha(\Omega) \) and \( A_\alpha^\dagger(\Omega) \). Then we consider three matrix elements. Necessary computations in the basis of eigenstates of free hamiltonian \( H_A \) are simple though a bit tedious, in some cases a suitable changes of summation indices is necessary. The results of these calculations are as follows
\[
\langle a \left| A_\beta(\Omega) \rho(t) \right| A_\alpha^\dagger(\Omega) \rangle \rho_{mn}(t) = \\
\sum_{m,n} \delta(\omega_{ma} - \Omega) \delta(\omega_{nb} - \Omega) \langle a \left| A_\beta \right| m \rangle \langle n \left| A_\alpha^\dagger \right| b \rangle \rho_{mn}(t), \tag{85a}
\]
\[
\langle a \left| A_\alpha^\dagger(\Omega) \right| A_\beta(\Omega) \rho(t) \rangle \rho_{mb}(t) = \\
\sum_{m,n} \delta(\omega_{an} - \Omega) \delta(\omega_{mn} - \Omega) \langle a \left| A_\alpha^\dagger \right| n \rangle \langle n \left| A_\beta \right| m \rangle \rho_{mb}(t), \tag{85b}
\]
\[
\langle a \left| \rho(t) A_\alpha^\dagger(\Omega) A_\beta(\Omega) \right| b \rangle = \\
\sum_{m,n} \delta(\omega_{mn} - \Omega) \delta(\omega_{bn} - \Omega) \langle m \left| A_\alpha^\dagger \right| n \rangle \langle n \left| A_\beta \right| a \rangle \rho_{am}(t). \tag{85c}
\]

The computed matrix elements are plugged into equation (84) and summation over frequency \( \Omega \) is performed. After some regrouping we find that
\[
\frac{d}{dt} \rho_{ab}(t) \bigg|_{d.} = \frac{1}{\hbar^2} \sum_{\alpha, \beta} \sum_{m,n} \left\{ \Gamma_{\alpha\beta}(\omega_{ma}) \left[ \delta(\omega_{nb} - \omega_{ma}) \langle a \left| A_\beta \right| m \rangle \langle b \left| A_\alpha \right| n \rangle \right] \rho_{mn}(t) \right. \\
- \frac{1}{2} \Gamma_{\alpha\beta}(\omega_{an}) \langle n \left| A_\beta \right| m \rangle \langle b \left| A_\alpha \right| a \rangle \right\} \rho_{mb}(t) \\
- \frac{1}{2} \Gamma_{\alpha\beta}(\omega_{mn}) \langle n \left| A_\beta \right| b \rangle \langle n \left| A_\alpha \right| m \rangle \rho_{am}(t) \bigg\}. \tag{86}
\]

Going further, we use the evenness of Kronecker delta in the first term, while the presence of the deltas in the second and third terms allows us to change arguments in the elements of matrix \( \Gamma_{\alpha\beta} \). Next, we denote
\[
K(am, bn) = \frac{1}{\hbar^2} \sum_{\alpha, \beta} \Gamma_{\alpha\beta}(\omega_{ma}) \langle a \left| A_\beta \right| m \rangle \langle b \left| A_\alpha \right| n \rangle, \tag{87}
\]
Due to these, we rewrite formula (86) as
\[
\frac{d}{dt} \rho_{ab}(t) \bigg|_{d.} = \sum_{m,n} \delta(\omega_{ma} - \omega_{nb}) K(am, bn) \rho_{mn}(t) \]
\[\quad - \frac{1}{2} \sum_{m,n} \delta(\omega_{mn} - \omega_{an}) K(nm, na) \rho_{mb}(t) \]
\[\quad - \frac{1}{2} \sum_{m,n} \delta(\omega_{bn} - \omega_{mn}) K(nb, nm) \rho_{am}(t). \tag{88}\]

Let us note the specific symmetry of this expression. Further analysis depends on whether the eigenfrequencies of the hamiltonian \(H_A\) are degenerate or not. We also note that Kronecker deltas in the second and third terms are correspondingly given as \(\delta(\omega_{mn} - \omega_{an}) = \delta(\omega_{ma})\) and \(\delta(\omega_{bn} - \omega_{mn}) = \delta(\omega_{bm})\), which allows one to perform summation over \(n\). However, one has to be careful because eigenfrequencies \(\omega_n\) can be degenerate.

### 5.5 Degenerate eigenfrequencies

To account for the possible degeneracies, let us write the hamiltonian of the considered system \(A\) in the following form
\[
H_A = \sum_{N} \hbar \omega_N \sum_{n=1}^{g_N} |Nn\rangle\langle Nn|, \tag{89}\]
where \(N\) is the main quantum number which distinguishes energy levels (energy multiplets), while \(n = 1, 2, \ldots, g_N\), are subsidiary quantum numbers. Is is obvious that \(\omega_N \neq \omega_M\) for \(N \neq M\). Certainly, the nondegenerate case follows immediately and it corresponds to \(g_N = 1\), then subsidiary quantum numbers are unnecessary and can be simply suppressed.

In the degenerate case single indices appearing in equation (88) must be replaced by corresponding pairs, for example \(a \rightarrow Aa\). Equation (88) is now rewritten as
\[
\frac{d}{dt} \rho_{AaBb}(t) \bigg|_{d.} = \sum_{Mm,Nn} \delta(\omega_{MA} - \omega_{NB}) K(AaMm, BbNn) \rho_{MmNn}(t) \]
\[\quad - \frac{1}{2} \sum_{Mm,Nn} \delta(\omega_{MN} - \omega_{AN}) K(NnMm, NnAa) \rho_{MmBb}(t) \]
\[\quad - \frac{1}{2} \sum_{Mm,Nn} \delta(\omega_{BN} - \omega_{MN}) K(NnBb, NnMm) \rho_{AaMm}(t). \tag{90}\]

As already noted, one immediately sees that \(\delta(\omega_{MN} - \omega_{AN}) = \delta(\omega_{MA}) = \delta_{MA}\) and similarly \(\delta(\omega_{BN} - \omega_{MN}) = \delta_{MB}\), where the last deltas are the simple Kronecker ones. The sum over \(M\) in the second term is trivial. We put \(M = A\) and we "land
within multiplet $A''$, hence we change $m = a''$. Analogously, in the second term $M = B$ and $m = b''$. Therefore, we have

$$\frac{d}{dt} \rho_{AaBb}(t) \bigg|_{d.} = \sum_{Mm} \sum_{Nn} \delta(\omega_{MA} - \omega_{NB}) \ K(AaMm, BbNn) \ \rho_{MmNn}(t)$$

$$- \frac{1}{2} \sum_{Nn} \sum_{a''} K(NnAa'', NnAa) \ \rho_{Aa''Bb}(t)$$

$$- \frac{1}{2} \sum_{Nn} \sum_{b''} K(NnBb, NnBb'') \ \rho_{AaBb''}(t). \quad (91)$$

In two last terms matrix elements do not depend on quantum numbers $Nn$, hence we can denote

$$\kappa(Aa, Bb) = \sum_{Nn} K(NnAa, NnBb). \quad (92)$$

This allows us to write equation (92) in the form

$$\frac{d}{dt} \rho_{AaBb}(t) \bigg|_{d.} = \sum_{Mm} \sum_{Nn} \delta(\omega_{MA} - \omega_{NB}) \ K(AaMm, BbNn) \ \rho_{MmNn}(t)$$

$$- \frac{1}{2} \sum_{a''} \kappa(Aa'', Aa) \ \rho_{Aa''Bb}(t) - \frac{1}{2} \sum_{b''} \kappa(Bb, Bb'') \ \rho_{AaBb''}(t). \quad (93)$$

Let us consider this equation in some more detail. First, we take $A = B$ (and correspondingly $b \rightarrow a'$). This yields the equation of motion for "quasi-population" matrix elements taken within just one energy multiplet. Then, the first term in right-hand side contains $\delta(\omega_{MA} - \omega_{NA}) = \delta(\omega_{MN}) = \delta_{MN}$. The sum over $N = M$ is trivial ($n \rightarrow m'$) and we have

$$\frac{d}{dt} \rho_{AaAa'}(t) \bigg|_{d.} = \sum_{Mm} \sum_{Nn} K(AaMm, Aa'Mm') \ \rho_{MmMm'}(t)$$

$$- \frac{1}{2} \sum_{a''} \kappa(Aa'', Aa) \ \rho_{Aa''Aa'}(t) - \frac{1}{2} \sum_{a''} \kappa(Aa', Aa'') \ \rho_{AaAa''}(t). \quad (94)$$

This equation connects "quasi-populations" with other ones. The first sum contains the term with $A = M$ and this term represents elastic (energy conserving) processes. The remaining terms (with $M \neq A$) corresponding to nonelastic transitions. In this case, the environment $B$ serves as a reservoir which gives or absorbs the energy. The terms in the second line describe the "escape" from multiplet $A$ to other ones.

To discuss coherences, we assume $A \neq B$, which implies $\omega_A \neq \omega_B$. The Kronecker delta in (93) can be rewritten as $\delta(\omega_{MA} - \omega_{NA}) = \delta(\omega_{MN} - \omega_{AB})$. Since $\omega_{AB} \neq 0$, we also get $\omega_{MN} \neq 0$. If we assume that all energy distances are different (that is $\omega_{AB} \neq \omega_{MN}$ for different pairs $A, B \neq M, N$) the considered delta can give unity.
only when $A = M$ and $B = N$ (which entails $m \to a'$ and $n \to b'$). Then, Eq. (93) reduces to

$$
\frac{d}{dt} \rho_{AaBb}(t) \bigg|_{d.} = \sum_{a'} \sum_{b'} K(\AAa', \BBb') \rho_{\AAa'Bb'}(t)
- \frac{1}{2} \sum_{a''} \kappa(\AAa'', \AAa) \rho_{\AAa'Bb'}(t)
- \frac{1}{2} \sum_{b''} \kappa(BBb'', \BBb) \rho_{Aa\BBb'}(t).
$$

(95)

So the coherences between two multiplets $A \neq B$ couple only with coherences from just these multiplets.

Obviously for the nondegenerate case "small" indices play no role – they can be suppressed. Then, instead of equation (94) for "quasi-populations" we get an equation for genuine populations

$$
\frac{d}{dt} \rho_{AA}(t) \bigg|_{d.} = \sum_{M} K(AM, AM) \rho_{MM}(t) - \kappa(A, A) \rho_{AA}(t).
$$

(96)

Similarly for coherences, Eq. (95) yields

$$
\frac{d}{dt} \rho_{AB}(t) \bigg|_{d.} = K(\AA, \BB) \rho_{AB}(t) - \frac{1}{2} \left[ \kappa(A, A) + \kappa(B, B) \right] \rho_{AB}(t).
$$

(97)

These examples indicate that ME for matrix elements of the reduced density operator possess quite a specific symmetry which probably can be further investigated. This, however, goes beyond the scope of the present work.

6 Auxiliary sections

6.1 Preservation of normalization

Any density operator, so also the reduced one for subsystem $A$ must be normalized, that is, we require that $\text{Tr}_A \{ \rho_A(t) \} = 1$. This has a simple consequence

$$
\frac{d}{dt} \text{Tr}_A \{ \rho_A(t) \} = \text{Tr}_A \left\{ \frac{d \rho_A(t)}{dt} \right\} = 0.
$$

(98)

Clearly the hamiltonian part (the commutator) preserves the trace, which follows from cyclic property. Hence we must check the second – dissipative part of our ME. One may ask at which stage of our derivation such a check should be made. In principle, this can be done at any stage. In this section we shall do so twice. Once for standard form (83), and for ME (93) in the energy basis.
Standard form

Taking ME in its standard form \((83)\) we need to compute the following trace

\[
S_T = \text{Tr}_A \left\{ \sum_{\alpha,\beta} \left[ \Gamma_{\alpha\beta}(\Omega) A_\beta(\Omega) \rho_A(t) A^\dagger_\alpha(\Omega) \right. \\
- \frac{1}{2} \Gamma_{\alpha\beta}(\Omega) A^\dagger_\alpha(\Omega) A_\beta(\Omega) \rho_A(t) \\
- \frac{1}{2} \Gamma_{\alpha\beta}(\Omega) \rho_A(t) A^\dagger_\alpha(\Omega) A_\beta(\Omega) \left. \right] \right\},
\]

and show that it vanishes, ie., \(S_T = 0\). The trace is a linear operation, so then

\[
S_T = \sum_{\Omega} \sum_{\alpha,\beta} \left[ \Gamma_{\alpha\beta}(\Omega) \text{Tr}_A \left\{ A_\beta(\Omega) \rho_A(t) A^\dagger_\alpha(\Omega) \right\} \right.
\\
- \frac{1}{2} \Gamma_{\alpha\beta}(\Omega) \text{Tr}_A \left\{ A^\dagger_\alpha(\Omega) A_\beta(\Omega) \rho_A(t) \right\} \\
- \frac{1}{2} \Gamma_{\alpha\beta}(\Omega) \text{Tr}_A \left\{ \rho_A(t) A^\dagger_\alpha(\Omega) A_\beta(\Omega) \right\} \right].
\]

(99)

Cyclic property allows one to see that all three traces are equal. Therefore, \(S_T = 0\) and we conclude that preservation of the normalization for ME in the standard form is proved.

ME in energy basis

In this case we check the trace preservation for Eq.\((94)\), with \(a' = a\). We need to compute

\[
S_T = \sum_{Aa} \sum_{Mm,m'} K(AaMm', AaMm') \rho_{MmMm'}(t)
\\
- \frac{1}{2} \sum_{Aa} \sum_{a''} \kappa(Aa'', Aa) \rho_{Aa''Aa}(t) - \frac{1}{2} \sum_{Aa} \sum_{a''} \kappa(Aa, Aa'') \rho_{AaAa''}(t).
\]

(101)

In the first term we use definition of the parameter \(\kappa\) (see \((92)\)). In the two next ones we notice that indices \(a\) and \(a''\) concern the same multiplet \(A\), so the summation range is also the same. We can interchange \(a \rightarrow a''\) and obtain

\[
S_T = \sum_{Mm,m'} \kappa(Mm, Mm') \rho_{MmMm'}(t)
\\
- \frac{1}{2} \sum_{Aa} \sum_{a''} \kappa(Aa, Aa'') \rho_{AaAa''}(t) - \frac{1}{2} \sum_{Aa} \sum_{a''} \kappa(Aa, Aa'') \rho_{AaAa''}(t).
\]

(102)

The second and third terms are identical and cancel out with the first one (names of summation indices are irrelevant). We have shown that in the energetic basis the trace of the reduced density operator for subsystem \(A\) is preserved. In other words, the derived ME preserves normalization.
6.2 Hermiticity of the reduced density operator

The next necessary property of any density operator is its hermiticity. If the equation of motion for \( \rho_A^\dagger(t) \) is identical with the similar equation for \( \rho_A(t) \), then the same equations must yield the same solutions, this means that \( \rho_A^\dagger(t) = \rho_A(t) \). Free evolution is given by the hamiltonian term \((-i/\hbar) [H_A + H_{LS}, \rho_A(t)]\) which poses no problems due to the commutator properties. One needs to investigate the dissipative part of ME. As in the previous section we perform such a check for ME in standard form and for the one in energy basis.

**Standard form**

We take the hermitian conjugate of the dissipative part of ME

\[
\frac{d}{dt} \rho_A^\dagger(t) \bigg|_d = + \frac{1}{\hbar^2} \sum_\Omega \sum_{\alpha,\beta} \left\{ \Gamma^*_{\alpha\beta}(\Omega) A_\alpha(\Omega) \rho_A(t) A_\beta(\Omega) 
\right. \\
\left. - \frac{1}{2} \Gamma^*_{\alpha\beta}(\Omega) [A_\beta(\Omega) A_\alpha(\Omega), \rho_A^\dagger(t)]_+ \right\},
\]

(103)

because conjugate anticommutator is equal to the anticommutator of conjugated operators. We know (see (75)) that matrix \( \Gamma_{\alpha\beta} \) is hermitian. Interchanging the indices \( \alpha \leftrightarrow \beta \) we get

\[
\frac{d}{dt} \rho_A^\dagger(t) \bigg|_d = + \frac{1}{\hbar^2} \sum_\Omega \sum_{\alpha,\beta} \left\{ \Gamma_{\alpha\beta}(\Omega) A_\beta(\Omega) \rho_A^\dagger(t) A_\alpha(\Omega) 
\right. \\
\left. - \frac{1}{2} \Gamma_{\alpha\beta}(\Omega) [A_\alpha(\Omega) A_\beta(\Omega), \rho_A(t)]_+ \right\},
\]

(104)

We see that the equation of motion for \( \rho_A^\dagger \) is formally identical with standard form (83) of ME. Thus, \( \rho_A^\dagger = \rho_A \) – hermiticity is preserved.

**ME in energetic basis**

Hermiticity of the density operator means that \( \rho_{AaBb} = \rho_{BbAa}^* \). It entails, that the equation of motion for the element \( \rho_{BbAa}^\dagger \) must be the same as for \( \rho_{AaBb} \). Starting from ME (93) we look for a corresponding equation for \( \rho_{BbAa}^* \). First we need to change the indices in (93) (remembering that corresponding changes must be made for summation indices in all terms) and then we perform complex conjugation. In this manner we find

\[
\frac{d}{dt} \rho_{BbAa}^\dagger(t) \bigg|_d = \sum_{Mm \, Nn} \delta(\omega_{MB} - \omega_{NA}) K^*(BbMm, AaNn) \rho_{MmNn}^\dagger(t) \\
- \frac{1}{2} \sum_{B'\prime} \kappa^*(Bb', Bb) \rho_{Bb'Aa}^\dagger(t) \\
- \frac{1}{2} \sum_{A''} \kappa^*(Aa, Aa'') \rho_{BbAa''}^\dagger(t).
\]

(105)
Next, we need to consider the conjugated quantities $K^*$ and $\kappa^*$. By definition (87)

$$
\delta(\omega_{MA} - \omega_{NB}) K(AaMm, BbNn) = \frac{1}{\hbar^2} \sum_{\alpha,\beta} \Gamma_{\alpha\beta} (\omega_{MA}) \langle Aa | A_{\beta} | Mm \rangle \langle Bb | A_{\alpha} | Nn \rangle^*.
$$

(106)

We take complex conjugates, use hermiticity of matrix $\Gamma_{\alpha\beta}$ and we notice that the presence of the Kronecker delta allows the change of the argument in $\Gamma$. Interchanging the summation indices $\alpha \leftrightarrow \beta$ we have

$$
\delta(\omega_{MA} - \omega_{NB}) K^*(AaMm, BbNn) = \frac{1}{\hbar^2} \sum_{\alpha,\beta} \Gamma_{\alpha\beta} (\omega_{NB}) \langle Bb | A_{\beta} | Nn \rangle \langle Aa | A_{\alpha} | Mm \rangle^*.
$$

(107)

Comparing this relation with definition (87) we see that

$$
\delta(\omega_{MA} - \omega_{NB}) K^*(AaMm, BbNn) = \delta(\omega_{MA} - \omega_{NB}) K(BbNn, AaMm).
$$

(108)

Next, we deal with the parameter $\kappa^*(Aa'', Aa)$. In the above relation we substitute $Aa \rightarrow Nn$, $Mm \rightarrow Aa''$, $Bb \rightarrow Nn$ and $Nn \rightarrow Aa$. Then

$$
\delta(\omega_{AN} - \omega_{AN}) K^*(NnAa'', NnAa) = \delta(\omega_{AN} - \omega_{AN}) K(NnAa, NnAa'').
$$

(109)

Obviously Kronecker deltas are equal to one, so they are unimportant. Using this result in the definition (92) of the parameter $\kappa$ we get

$$
\kappa^*(Aa'', Aa) = \sum_{Nn} K^*(NnAa'', NnAa) = \sum_{Nn} K(NnAa, NnAa'') = \kappa(Aa, Aa'').
$$

(110)

Returning to the analysis of formula (105), we use the proven relations (108) and (110). At the same time, in the first term in the right hand side we interchange the summation indices $Mm \leftrightarrow Nn$. Moreover, we recall that Kronecker delta is even. Thus, we have

$$
\frac{d}{dt} \rho_{aA}^{bB}(t) \bigg|_{t=0} = \sum_{Mm} \sum_{Nn} \delta(\omega_{MA} - \omega_{NB}) K(AaMm, BbNn) \rho_{NnMm}^{aA}(t)
\quad - \frac{1}{2} \sum_{Bb''} \kappa(Bb, Bb'') \rho_{Bb''Aa}^{Bb}(t) - \frac{1}{2} \sum_{Aa''} \kappa(Aa', Aa) \rho_{BbAa''}^{Bb}(t).
$$

(111)

Comparing this result with Eq. (93) we find that when we replace $\rho_{AaBb}$ by $\rho_{BbAa}$ (consequently in all the terms) then we will arrive at (111). This equation is formally identical with Eq. (93), hence $\rho = \rho^\dagger$, what we intended to show. Our ME preserves hermiticity of the reduced density operator of subsystem $A$. 

S.K, J.C-K
6.3 Reduced density operator in interaction picture

In this section we will show that the reduction of the density operator is invariant with respect to the choice of the picture. The definition (6) of the reduced density operator and (9) for the transformation to the interaction picture imply that the operator \( \rho_A(t) \) (in the Schrödinger picture) is expressed as

\[
\rho_A(t) = \text{Tr}_B \{ \rho_{AB}(t) \} = \text{Tr}_B \left\{ e^{-iH_0t/\hbar} \tilde{\rho}_{AB}(t) e^{iH_0t/\hbar} \right\}.
\]

(112)

We note that the free evolution of each of the subsystems written as

\[
|\varphi_A(0)\rangle \otimes |\psi_B(0)\rangle \longrightarrow |\varphi_A(t)\rangle \otimes |\psi_B(t)\rangle,
\]

(113)

can be expressed with the aid of the operator

\[
\exp \left( -\frac{i}{\hbar} H_0 t \right) = \exp \left( -\frac{i}{\hbar} H_A t \right) \otimes \exp \left( -\frac{i}{\hbar} H_B t \right),
\]

(114)

because both hamiltonians are fully independent and commute. In Eq.(112) we compute the trace only over reservoir variables, so we can write

\[
\rho_A(t) = e^{-iH_A t/\hbar} \text{Tr}_B \left\{ e^{-iH_B t/\hbar} \tilde{\rho}_{AB}(t) e^{iH_B t/\hbar} \right\} e^{iH_A t/\hbar}.
\]

(115)

Cyclic property of the trace yields

\[
e^{iH_A t/\hbar} \rho_A(t) e^{-iH_A t/\hbar} = \text{Tr}_B \{ \tilde{\rho}_{AB}(t) \}.
\]

(116)

Left hand side represents the reduced density operator in the interaction picture (it depends solely on the variables of the subsystem \( A \)). Hence, we have

\[
\tilde{\rho}_A(t) = \text{Tr}_B \{ \tilde{\rho}_{AB}(t) \}.
\]

(117)

This is formally identical with the definition of the reduced density operator in the Schrödinger picture. The relation between the reduced density and the total one is the same in both pictures. In other words, reduction of the operator \( \rho_A(t) = \text{Tr}_B \{ \rho_{AB}(t) \} \) is invariant with respect to the change of the pictures.

6.4 Existence of two time scales. Discussion of approximations

In this section we follow and (hopefully) try to elucidate the discussion presented by Cohen-Tannoudji et al [6]. The previously given remarks apply also here, so we again refrain from frequent citations.

Order of magnitude of time \( T_A \)

The key role in our considerations is played by the assumption (17). This is the requirement

\[
\tau_B \ll \Delta t \ll T_A.
\]

(118)
In other words we assume that there exist two, quite distinct, time scales. Firstly, let us try to estimate the time $T_A$ which characterizes the evolution of system $A$ due to the interaction with reservoir. To find such an estimate we use Eq. (32), that is

$$\Delta \tilde{\rho}_A(t) = \left(\frac{1}{i\hbar}\right)^2 \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \text{Tr}_B \left\{ \begin{array}{c} \tilde{V}_{AB}(t_1), \quad [\tilde{V}_{AB}(t_2), \tilde{\rho}_A(t) \otimes \bar{\sigma}_B] \end{array} \right\},$$  

(119)

where we employed the introduced properties of the reservoir. We also recall that the main contribution to the integrals comes from a thin belt (of width $\tau_B$ lying below the diagonal $t_1 = t_2$, see Fig. 1 and its discussion). This allows us to estimate the integrand as follows

$$\text{Tr}_B \left[ \tilde{V}_{AB}(t_1), \quad [\tilde{V}_{AB}(t_2), \tilde{\rho}_A(t) \otimes \bar{\sigma}_B] \right] \sim \tilde{\rho}_A \text{Tr}_B \left\{ \tilde{V}^2 \bar{\sigma}_B \right\} = V^2 \tilde{\rho}_A.$$  

(120)

Hence, left hand side of Eq. (119) is estimated by

$$\frac{\Delta \tilde{\rho}_A}{\Delta t} \sim \frac{1}{\hbar^2} \tau_B V^2 \tilde{\rho}_A,$$  

(121)

because the area of the integration region is estimated by the product $\tau_B \Delta t$ (area of the belt under the diagonal $t_1 = t_2$). Introduced parameter $V$ characterizes the "strength" of the interaction between the reservoir and system $A$. The factor which multiplies $\tilde{\rho}_A$ in (121) has (according to (16)) the sense of the inverse of time $T_A$. Therefore, we obtain an estimate

$$\frac{1}{T_A} \sim \frac{V^2 \tau_B}{\hbar^2}, \quad \text{or} \quad T_A \sim \frac{\hbar^2}{V^2 \tau_B}.$$  

(122)

**Condition for existence of two time scales**

What is the condition of the existence of two time scales? The estimate of $T_A$ given in (122) allows us to find such a condition. Let us look upon condition $\tau_B \ll T_A$ more carefully and introduce the estimate (122). This yields

$$\tau_B \ll \frac{\hbar^2}{V^2 \tau_B} \quad \Rightarrow \quad \frac{V \tau_B}{\hbar} \ll 1.$$  

(123)

The last inequality is the sought condition of existence of two time scales. If we denote $\Omega_{AB} = V/\hbar$, then we can write $\Omega_{AB} \tau_B \ll 1$. So the interaction must be characterized by such Bohr frequency $\Omega_{AB}$ that during the time interval of magnitude of $\tau_B$ its influence on system $A$ is negligibly small.
Justification of weak coupling approximation

We already mentioned (see the discussion of Eq. (14)), that it is possible to iterate von Neumann equation – accounting for higher order corrections would increase accuracy. We can estimate these higher order terms in the same manner as done just above. For example, for the third order term we have

\[
\frac{\Delta \tilde{\rho}_A}{\Delta t} \mid _{(3)} \sim \frac{V^3}{\hbar^3} \tau_B^2 \tilde{\rho}_A, \tag{124}
\]

because times \(t_1, t_2\) and \(t_3\) must be close to each other (with accuracy of the order of \(\tau_B\)). Then the region of integration has volume of the order of \(\tau_B^2 \Delta t\). Due to Eq. (122) we get

\[
\frac{\Delta \tilde{\rho}_A}{\Delta t} \mid _{(3)} \sim \frac{V \tau_B}{\hbar} \cdot \frac{1}{T_A} \tilde{\rho}_A \ll \frac{1}{T_A} \tilde{\rho}_A, \tag{125}
\]

where the last inequality follows from (123). The obtained estimate shows that the third order iteration (and similarly higher ones) are indeed negligible. Obviously this holds provided the condition (123) is true and ensures the existence of two distinct time scales.

Neglecting \(\rho_{\text{corel}}\) (Born approximation)

Moving from Eq. (14) to (32) we have neglected initial correlations between systems \(A\) and \(B\). These correlations built up at earlier moments \(t' < t\). This corresponds to the assumption that at some earlier moment \(t_0\) (\(t_0 < t\)) both systems were uncorrelated. This happens, for example, when the interaction was switched on at an instant \(t_0\). So the correlations described by \(\tilde{\rho}_{\text{corel}}\) need time \(t - t_0\) to appear. If the correlations exist \((\tilde{\rho}_{\text{corel}} \neq 0)\) then averaging of the term linear in interaction (as in expression (31)) would not give zero. Hence, \(\tilde{\rho}_{\text{corel}} \neq 0\) would result in the appearance of the linear term. Moreover, this would also automatically modify the quadratic term in (33). Let us estimate the magnitude of this modification (which is due to earlier interaction)

\[
\frac{\Delta \tilde{\rho}_A}{\Delta t} \sim \frac{1}{\Delta t} \left( \frac{1}{ih} \right)^2 \int_{-\infty}^{t} dt_1 \int_{t}^{t+\Delta t} dt_2 \langle \tilde{V}_{AB}(t_1)\tilde{V}_{AB}(t_2) \rangle_B. \tag{126}
\]

The integrand contains correlation functions of the reservoir. Hence the integrand would be practically zero for \(|t_1 - t_2| \geq \tau_B\). The integration runs effectively from \(t - \tau_B\) to \(t + \tau_B\). Therefore, using condition (122), we estimate

\[
\frac{\Delta \tilde{\rho}_A}{\Delta t} \sim \frac{1}{\Delta t} \cdot \frac{V^2}{\hbar^2} \tau_B^2 = \frac{V^2 \tau_B}{\hbar^2} \cdot \frac{\tau_B}{\Delta t} = \frac{1}{T_A} \cdot \frac{\tau_B}{\Delta t}, \tag{127}
\]

as the integrals are nonzero within the interval of the length of the order of \(\tau_B\). If \(\tau_B \ll \Delta t\) then the correction is small (main contribution to the evolution of \(\tilde{\rho}_A\)
is of the order of $1/T_A$, which is quite larger). The key assumption that $\tau_B \ll \Delta t$ allows us to conclude that the correlations between system $A$ and $B$ which were built before moment $t$ do not significantly change the evolution of $\tilde{\rho}_A(t)$, their influence is restricted to the moments from a very short interval $(t, t - \tau_B)$. New correlations, within a much longer interval $(t, t + \Delta t)$, are building up and have an effect on the evolution of $\tilde{\rho}_A(t)$. Initial correlations have small significance and hence it is justified to neglect them.

**Discussion of the secular approximation**

Secular approximation consists in replacing the function $F(\Omega' - \Omega)$ (defined in (66)) in (68) by Kronecker delta, which leads to Eq.(70). Our discussion of this replacement does not rise any doubts when $|\Omega' - \Omega| \ll (\Delta t)^{-1}$, because then $F(\Omega' - \Omega)$ is practically unity. On the other hand for $|\Omega' - \Omega| \gg (\Delta t)^{-1}$ the function $F(\Omega' - \Omega)$ is practically zero. The only problem is to justify the neglecting of the terms for which $|\Omega' - \Omega| \sim (\Delta t)^{-1}$.

To explain this point, first use the fact that the free evolution of matrix elements $\rho_{ab}$ is governed by

$$
\frac{d}{dt} \rho_{ab}^{(F)} = -\frac{i}{\hbar} \langle a | [H_A, \rho^{(F)}] | b \rangle = -i\omega_{ab}\rho_{ab}^{(F)},
$$

(128)

where the small Lamb shift (due to $H_{LS}$) is ignored. The solution is simple

$$
\rho_{ab}^{(F)}(t) = e^{-i\omega_{ab}t}\rho_{ab}^{(F)}(0).
$$

(129)

Now, we analyze the dissipative term which is given by (88). We do not discuss the nuances connected with possible degeneracies. Obviously, we can write

$$
\rho_{mb} = \sum_k \delta_{bk}\rho_{mk} \quad \text{and} \quad \rho_{am} = \sum_k \delta_{ak}\rho_{km},
$$

(130)

which we use in (88). We also interchange indices $k \leftrightarrow n$ in the second term and similarly, in the third one we first interchange $m \leftrightarrow n$ and then $k \leftrightarrow m$. The result is

$$
\left. \frac{d}{dt} \rho_{ab}(t) \right|_d = \sum_{m,n} \delta(\omega_{ma} - \omega_{nb}) K(am, bn) \rho_{mn}(t)

- \frac{1}{2} \sum_{k,m,n} \delta_{bn} \delta(\omega_{mk} - \omega_{ak}) K(km, ka) \rho_{mn}(t)

- \frac{1}{2} \sum_{k,m,n} \delta_{am} \delta(\omega_{bk} - \omega_{ak}) K(kb, kn) \rho_{mn}(t).
$$

(131)

We note that $\delta_{bn}$ implies $b = n$, and then $\omega_{nb} = 0$. Therefore

$$
\delta_{bn} \delta(\omega_{mk} - \omega_{ak}) = \delta_{bn} \delta(\omega_{ma}) = \delta_{bn} \delta(\omega_{ma} - \omega_{nb}),
$$

(132)
since $\omega_{nb} = 0$ and changes nothing. Similarly we have

$$\delta_{am} \delta(\omega_{bk} - \omega_{nk}) = \delta_{am} \delta(-\omega_{nb}) = \delta_{bn} \delta(\omega_{ma} - \omega_{ab}).$$

(133)

Finally, we note that $\delta(\omega_{ma} - \omega_{nb}) = \delta(\omega_{ab} - \omega_{mn})$, because Kronecker delta is even. After these manipulations Eq. (131) can be written as

$$\frac{d}{dt} \rho_{ab}(t) \bigg|_{d.} = \sum_{m,n} \delta(\omega_{ab} - \omega_{mn}) \left\{ K(am, bn) - \frac{1}{2} \delta_{bn} \sum_{k} K(km, ka) 
- \frac{1}{2} \delta_{am} \sum_{k} K(kb, kn) \right\} \rho_{mn}(t).$$

(134)

The expression in braces is denoted as $M_{am, bn}$ and we have

$$\frac{d}{dt} \rho_{ab}(t) \bigg|_{d.} = \sum_{m,n} \delta(\omega_{ab} - \omega_{mn}) M_{am, bn} \rho_{mn}(t).$$

(135)

This is a specific form of ME, but useful in the discussion. However, in the degenerate case some care must be exercised and renewed considerations might be necessary.

We proceed to the discussion of conditions and/or possibilities of neglecting the terms for which $|\Omega' - \Omega| \sim (\Delta t)^{-1}$. Interaction with the reservoir certainly modifies the free evolution of $\rho_{ab}^{(F)}(t) = e^{-i\omega_{ab}t} \rho_{ab}^{(F)}(0)$. If Bohr frequencies of the oscillating elements $\rho_{ab}$ are such that $|\omega_{ab} - \omega_{mn}| \gg 1/T_A$, then mutual couplings between these elements are quickly averaged to zero (interfere destructively) before time $T_A$ elapses and before the interaction has enough time to affect the evolution. In other words, if $|\omega_{ab} - \omega_{mn}|$ differs much from $1/T_A$ then the coupling between corresponding matrix elements will have small (weak) effect. This is the situation similar to the one encountered in perturbation theory. Namely, when the energies $|E_a - E_b| \gg V_{ab} = \langle a | V | b \rangle$ then the perturbation has small (usually negligible) effect.

Since, by assumption $T_A \gg \Delta t$ the discussed situation corresponds, in fact, to the relation $|\omega_{ab} - \omega_{cd}| \sim (\Delta t)^{-1}$. This, in turn means, that such terms have little influence on the evolution of the operator $\rho_A(t)$. Such terms are neglected while passing from Eq. (68) to (70). Thus the last of our approximations is justified.

### 6.5 $V_{AB} = V_{AB}^\dagger$ - nonhermiticity of operators $A_\alpha$ i $X_\alpha$

In our considerations we have adopted the interaction hamiltonian between the system $A$ and reservoir $B$ in the form $V_{AB} = \sum_\alpha A_\alpha \otimes X_\alpha$, where operators $A_\alpha$ and $X_\alpha$ do not have to be hermitian. Certainly, the full interaction hamiltonian must be hermitian, so we conclude that it must contain operators $A_\alpha$, $X_\alpha$ and their hermitian conjugates $A_\alpha^\dagger$, $X_\alpha^\dagger$. Constructing linear combinations we can always transform the interaction hamiltonian into $V_{AB} = \sum_\alpha A_\alpha \otimes X'_\alpha$, where the primed operators are hermitian.

We shall illustrate this with a simple example. Let the interaction hamiltonian be of the form

$$V_{AB} = A \otimes X^\dagger + A^\dagger \otimes X,$$

(136)
where operators $A$ and $X$ are nonhermitian, while the full hamiltonian is clearly hermitian. We define new operators

$$
q = \frac{1}{\sqrt{2}}(A + A^\dagger), \quad Q = \frac{1}{\sqrt{2}}(X + X^\dagger),
$$

$$
p = \frac{i}{\sqrt{2}}(A - A^\dagger), \quad P = \frac{i}{\sqrt{2}}(X - X^\dagger),
$$

(137)

which are evidently hermitian. Expressing operators $A$, $X$ and their conjugates via the new ones, we obtain

$$
V_{AB} = \frac{1}{2}(q - ip) \otimes (Q + iP) + \frac{1}{2}(q + ip) \otimes (Q - iP)
$$

$$
= q \otimes Q + p \otimes P.
$$

(138)

This interaction hamiltonian is expressed as a sum of products of hermitian operators. Hence construction of the interaction hamiltonian with nonhermitian operators is allowed. One can always build necessary combinations. However, in some practical applications it is much more convenient to use nonhermitian operators than the linear combinations.

### 6.6 Vanishing average $\langle X_\alpha \rangle_B$

In the main part of the lecture we assumed that Eq.(29) holds, that is the average $\langle X_\alpha \rangle_B \equiv \text{Tr}_B \{ X_\alpha \rho_B(t) \} = 0$. We have stated that it is not really restrictive. We will show that it is true. This is so, because we can always shift the energy scale. To see this, let us write

$$
V_{AB}' = \sum_\alpha A_\alpha \otimes (X_\alpha - \langle X_\alpha \rangle_B)
$$

$$
= \sum_\alpha A_\alpha \otimes X_\alpha - \sum_\alpha \langle X_\alpha \rangle_B (A_\alpha \otimes 1_B),
$$

(139)

where $\langle X_\alpha \rangle_B = \text{Tr}_B \{ \bar{\sigma}_B X_\alpha \}$ is a number not necessarily equal to zero. Then we have

$$
\langle V_{AB}' \rangle_B = \sum_\alpha A_\alpha (\langle X_\alpha \rangle_B - \langle X_\alpha \rangle_B) = 0,
$$

(140)

which holds no matter whether numbers $\langle X_\alpha \rangle_B$ are zeroes or not. Full hamiltonian can then be written as

$$
H_{AB} = H_A \otimes 1_B + 1_A \otimes H_B + V_{AB}
$$

$$
= H_A \otimes 1_B + 1_A \otimes H_B + V_{AB}' + \sum_\alpha \langle X_\alpha \rangle_B (A_\alpha \otimes 1_B)
$$

$$
= [H_A + \sum_\alpha (X_\alpha)_{BA} A_\alpha] \otimes 1_B + 1_A \otimes H_B + V_{AB}'.
$$

(141)
Rescaled interaction term (the last one) has zero average (as in (140)). This is achieved by the redefinition of the energy scale in system $A$ – via redefinition of the hamiltonian $H_A$. We conclude that the assumption that the averages (29) vanish is not really restrictive, but simplifies the computation.

6.7 Commutators of operators $A_\alpha(\Omega)$

In the main sections we have introduced the operators $A_\alpha(\Omega)$ defined by relation (35). The hamiltonian of system $A$ is of the form $H_A = \sum_n \hbar \omega_n |n\rangle \langle n|$. It is not difficult to find the commutator $[H_A, A_\alpha(\Omega)]$. Directly from the definitions we obtain

$$
[H_A, A_\alpha(\Omega)] = \left[ \sum_n \hbar \omega_n |n\rangle \langle n|, \sum_{a,b} \delta(\omega_{ba} - \Omega) |a\rangle \langle a| A_\alpha |b\rangle \langle b| \right]
$$

$$
= \sum_{a,b} \hbar (\omega_a - \omega_b) \delta(\omega_{ba} - \Omega) |a\rangle \langle a| A_\alpha |b\rangle \langle b| = - \hbar \Omega A_\alpha(\Omega),
$$

(142)

which ends the calculation. Conjugation changes sign, so that

$$
[H_A, A_\alpha^\dagger(\Omega)] = \hbar \Omega A_\alpha^\dagger(\Omega).
$$

(143)

Heisenberg equation of motion follows from formula (142), and it is

$$
i\hbar \frac{d}{dt} A_\alpha^{(H)}(\Omega) = [A_\alpha^{(H)}(\Omega), H_A] = \hbar \Omega A_\alpha^{(H)}(\Omega).
$$

(144)

After integration we obtain $A_\alpha^{(H)}(\Omega) = e^{i\Omega t} A_\alpha(\Omega)$ which agrees with (44). Finally, we present one more relation

$$
[H_A, A_\alpha^\dagger(\Omega) A_\beta(\Omega)] = A_\alpha^\dagger(\Omega) [H_A, A_\beta(\Omega)]
$$

$$
+ [H_A, A_\alpha^\dagger(\Omega)] A_\beta(\Omega) = 0,
$$

(145)

which follows immediately from the derived results.

6.8 Explicit form of correlation functions $\tilde{G}_{\alpha\beta}(\tau)$

Correlation function of the reservoir was defined in (47) or (53). By assumption, reservoir hamiltonian $H_B$ and the corresponding density operator $\tilde{\sigma}_B$ commute, so they have a common set of complete and orthonormal eigenstates $|z\rangle$. Let us calculate the trace in (53) in the chosen basis

$$
\tilde{G}_{\alpha\beta}(\tau) = \text{Tr}_B \left\{ \tilde{X}_\alpha^\dagger(\tau) X_\beta \tilde{\sigma}_B \right\} = \text{Tr}_B \left\{ e^{iH_B \tau / \hbar} X_\alpha^\dagger e^{-iH_B \tau / \hbar} X_\beta \tilde{\sigma}_B \right\}
$$

$$
= \sum_{z,\xi} \langle z | e^{iH_B \tau / \hbar} X_\alpha^\dagger e^{-iH_B \tau / \hbar} | \xi \rangle \langle \xi | X_\beta \tilde{\sigma}_B | z \rangle.
$$

(146)
In Eq. (22) we denoted the eigenvalues of $\bar{\sigma}_B$ by $p(z)$, hence

$$G_{\alpha\beta}(\tau) = \sum_{z,\xi} p(z) e^{i\omega_{z\xi}\tau} \langle z | X_\alpha^\dagger | \xi \rangle \langle \xi | X_\beta | z \rangle,$$

(147)

with $\omega_z = E_z/h$, and $\omega_{z\xi} = \omega_z - \omega_\xi$.

Expression (147) shows that the correlation function $G_{\alpha\beta}(\tau)$ is a complicated superposition of functions which oscillate with Bohr frequencies $\omega_{z\xi}$. Reservoir is assumed to be large, the discussed frequencies are densely spaced (quasi-continuous). If time $\tau$ is sufficiently large the oscillations interfere destructively (average out to zero). We can expect that reservoir correlation function decay quickly when time $\tau = t_1 - t_2$ increases. Characteristic decay time is denoted by $\tau_B$ and assumed to be, by far, the shortest time characterizing the system $A + B$. When $\tau > \tau_B$ the correlation may be neglected.

## 7 Summary

In this summary we describe practical steps needed in the construction of the ME for specified physical systems.

The first step consists in precise definition of the system $A$ and of the reservoir $B$. We need to specify their free hamiltonians $H_A$ and $H_B$ and (at least sometimes) their eigenenergies and eigenstates. Then we define the interaction hamiltonian in the form

$$V_{AB} = \sum_{\alpha} A_\alpha \otimes X_\alpha = \sum_{\alpha} A_\alpha^\dagger \otimes X_\alpha^\dagger,$$

(148)

where $A_\alpha$, $X_\alpha$ are (correspondingly) operators of system $A$ and reservoir. We stress that these operator need not be (separately) hermitian. It suffices that the full interaction hamiltonian is hermitian. We also need to specify the density operator $\bar{\sigma}_B$ describing the state of the reservoir. It is worth remembering that operator $H_B$ and $\bar{\sigma}_B$ commute. This implies that the reservoir is in the stationary state. In the second step of ME construction we build (identify) the following operators

$$A_\alpha(\Omega) = \sum_{a,b} \delta(\omega_{ba} - \Omega) | a \rangle \langle a | A_\alpha | b \rangle \langle b |.$$

(149)

The following matrix elements are computed in the third step

$$W_{\alpha\beta}(\Omega) = \int_0^\infty d\tau e^{i\Omega\tau} \bar{G}_{\alpha\beta}(\tau) = \int_0^\infty d\tau e^{i\Omega\tau} \text{Tr}_B \{ \bar{X}_\alpha(\tau) X_\beta \bar{\sigma}_B \}. $$

(150)

They are seen to be partial Fourier transform of the reservoir correlation functions. Reservoir operators are taken in the interaction picture

$$\bar{X}_\alpha(t) = e^{iH_B t/h} X_\alpha e^{-iH_B t/h}.$$

(151)
Coefficients $W_{\alpha\beta}(\Omega)$ are then employed to construct two hermitian matrices

$$\Gamma_{\alpha\beta}(\Omega) = W_{\alpha\beta}(\Omega) + W_{\beta\alpha}(\Omega),$$

$$\Delta_{\alpha\beta}(\Omega) = \frac{1}{2i} \left[ W_{\alpha\beta}(\Omega) - W_{\beta\alpha}(\Omega) \right].$$  \hspace{1cm} (152)

We note that $\Gamma_{\alpha\beta}(\Omega)$ is a positive-definite matrix and can be computed directly as Fourier transform

$$\Gamma_{\alpha\beta}(\Omega) = \int_{-\infty}^{\infty} d\tau e^{i\Omega \tau} \text{Tr}_B \{ \bar{\tilde{X}}_{\alpha}^{\dagger}(\tau)X_{\beta}\sigma_B \} = \int_{-\infty}^{\infty} d\tau e^{i\Omega \tau} \bar{G}_{\alpha\beta}(\tau).$$  \hspace{1cm} (153)

Parameters $\Gamma_{\alpha\beta}(\Omega)$, in practical applications, are more important than $\Delta_{\alpha\beta}(\Omega)$. Explanation will be given later. The separate expression for elements $\Delta_{\alpha\beta}(\Omega)$ is

$$\Delta_{\alpha\beta}(\Omega) = \frac{1}{2i} \left[ \int_{0}^{\infty} d\tau e^{i\Omega \tau} \text{Tr}_B \{ \bar{\tilde{X}}_{\alpha}^{\dagger}(\tau)X_{\beta}\sigma_B \} - \int_{0}^{\infty} d\tau e^{-i\Omega \tau} \text{Tr}_B \{ X_{\alpha}^{\dagger}\bar{\tilde{X}}_{\beta}(\tau)\sigma_B \} \right].$$  \hspace{1cm} (154)

Hence, calculation of coefficients $W_{\alpha\beta}(\Omega)$ can be usually omitted.

Final construction of the proper ME is the fourth and the last step. The above given quantities allow us to write the ME as

$$\frac{d}{dt} \rho_A(t) = -\frac{i}{\hbar} [H_A + H_{LS}, \rho_A(t)] + \frac{1}{\hbar^2} \sum_{\Omega} \sum_{\alpha,\beta} \Gamma_{\alpha\beta}(\Omega) \left\{ A_{\beta}(\Omega) \rho_A(t) A_{\alpha}^{\dagger}(\Omega) \right. \left. - \frac{i}{2} \left[ A_{\alpha}^{\dagger}(\Omega) A_{\beta}(\Omega), \rho_A(t) \right] \right\}_+, $$

where the so-called Lamb-shift hamiltonian $H_{LS}$ is given as

$$H_{LS} = \frac{1}{\hbar} \sum_{\Omega} \sum_{\alpha,\beta} \Delta_{\alpha\beta}(\Omega) A_{\alpha}^{\dagger}(\Omega) A_{\beta}(\Omega).$$  \hspace{1cm} (156)

Energy shifts of the system $A$ which are due to the presence of $H_{LS}$ in the hamiltonian part, are usually quite small and frequently negligible. This explains why the role of matrix $\Delta_{\alpha\beta}$ is usually less important than that of matrix $\Gamma_{\alpha\beta}$.

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