The theory of open localized quantum systems in representation of the effective Hamiltonian

A M Basharov
Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Russia
National Research Centre «Kurchatov Institute», 123182 Moscow, Russia
E-mail: basharov@gmail.com; http://basharov.me

Abstract. The paper substantiates the necessity of using the effective Hamiltonian in describing open optical systems.

1. Introduction
Many problems of physics and information theory are reduced to solving the kinetic equation for the density matrix of an open system. This equation is also referred to as master equation. It owes its origin due to separating a fairly independent subsystem from a large system, namely a subsystem, which retains its individual characteristics in case of weak interaction with its environment. This subsystem is called an open system, and its impact on the environment, as a rule, does not change the environment state. Examples of an open system are an excited atom in a surrounding vacuum electromagnetic field, photons of a microresonator mode coupled at the interface with photons of an electromagnetic field, etc.

Typically, the interaction of an open system is small and is characterized by the Markovian property. Otherwise, it would not make sense to describe an open system as an independent object. It follows from the Markovian property that the effect of an open system on the environment does not change the environment state, with no memory of the effect at previous times when the environment affects the system. In other words, the Markovian property is a stochastic Cauchy condition, i.e. further dynamics of an open system is statistically determined by the system state only at a given moment in time.

If the initial environment state is not entangled with the initial state of an open system and is not in a squeezed state, then in the Markov approximation the kinetic equation for the density matrix has a universal form, which is traditionally designated as the Lindblad form [1-3]:

$$\frac{d\rho^S(t)}{dt} = \gamma [\rho^S(t), H^\text{eff}_{S} S(t)] - \Gamma \rho^S(t), \quad \Gamma \rho^S(t) = \sum_{i=1}^{N} \Gamma_i \rho^S(t),$$

(1)

$$\Gamma_i \rho^S(t) = -\frac{i}{2} [\rho^S(t), H^L_{S-S} (t)] - \gamma \gamma_i \rho^S(t) L_i - \gamma \gamma_i \rho^S(t) (n_i + 1) L_i^+ +$$

$$+ \gamma (\frac{1}{2} (n_i + 1) L_i L_i^+ + \frac{i}{2} n_i L_i^+ L_i^+ \rho^S(t) + \rho^S(t) \gamma (\frac{1}{2} (n_i + 1) L_i L_i^+ + \frac{i}{2} n_i L_i^+ L_i^+)).$$

(2)

The $\Gamma$ operator is known to be a relaxation operator of an open system. The index $i$ lists all types of relaxation channels due to interaction with various components of the environment. Each relaxation channel has its own Lindblad operators $L_i$, $L_i^+$ and $H^L_{S-S} (t)$ describing the characteristics of the

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
spectrum of an open system, which are highly visible as the intrinsic emission of an open system (if any) in the form of broadening and shift of the spectral line. The value \( n_i \) indicates the characteristic density of excitations of the \( i \)-th component of the environment, which is determined by the temperature \( T \) in the state of thermodynamic equilibrium of the medium. Moreover, different components of the environment are meant as different thermal baths. If the thermal baths are spatially separated from each other, then they can be characterized by their temperatures \( T_i \).

We define the time argument explicitly to emphasize that the Dirac picture shows everything in the interaction representation. Finally, \( H^{eff-S}(t) \) is the effective Hamiltonian of an open system.

What is important is that the majority of research works on open systems represent the kinetic equation (1) as a source for further consideration of the dynamics of an open system and for further study of its behavior in various fields, including limiting or particular cases. Moreover, the form of the Lindblad operators is postulated. Considering the dynamics of an open system often goes beyond the scope of this type of kinetic equation, leading to erroneous results. The present paper discusses and substantiates the basic principle in physical laws, which should be taken into account when deriving the kinetic equation for an arbitrary open optical system.

2. A distinctive character of treating quantum open systems in optics

In optics, the general Hamiltonian of an open system and its environment \( H \) consists of the Hamiltonian of an isolated open system \( H^{Sys} \), the Hamiltonian \( H^{Env} \) of its environment and the interaction Hamiltonian \( V^{Sys-Env} : H = H^{Sys} + H^{Env} + V^{Sys-Env} \). An open quantum system is characterized by a discrete spectrum in the Hamiltonian \( H^{Sys} \). As a rule, the environment of an open system is multimode, with its spectrum having a continuous component. Regardless of the specific structure of the Hamiltonian of an open system, the operator of its interaction with the environment contains two different groups of terms in the case of a quantum open system. The terms of one group have factors containing exponentials of the form \( \exp[\pm i(\omega \pm \omega_0)t] \). Here the frequencies \( \omega \) are related to the environment and to the continuous spectrum, with the frequencies \( \omega_0 \) characterizing an open system. Such terms vary rapidly in time compared to the ones that do not contain these factors. There are also terms with factors \( \exp[\pm i(\omega - \omega_0)t] \) where the frequencies \( \omega \) are close to the frequencies of the discrete spectrum of the open system due to the fact that the environment spectrum is continuous, so that if there are no spectral features in the environment spectrum (for example, band gaps), then there are spectral regions where the resonance condition \( \omega \approx \omega_0 \) is fulfilled. This group of terms slowly changes in time. Further we will designate it as the terms that slowly change in time. It should be emphasized that similar terms with the factor \( \exp[\pm i(\omega - \omega_0)t] \), where the condition \( \omega \approx \omega_0 \) is not satisfied, i.e. \( \omega \) is far enough from \( \approx \omega_0 \), are rapidly changing in time. In other words, rapidly time-changing terms are referred to as anti-rotating terms, with slowly time-changing terms being the rotating ones. These groups of terms correspond to interaction processes, which are defined as nonresonant and resonant processes. In this context, it would be reasonable to emphasize that there are nonresonant processes observed in any interaction in the given situations, i.e. the general Hamiltonian always has rapidly time-changing terms while an open system and its environment being described.

For each particular open quantum system, it would be more convenient to divide into rapidly and slowly varying terms in the interaction representation (the Dirac picture). According to the picture, the operators are conventionally derived from the operators of the Schrödinger picture

\[
V^{Sys-Env}(t) = \exp(i(H^{Sys} + H^{Env})t/\hbar)V^{Sys-Env}\exp(-i(H^{Sys} + H^{Env})t/\hbar).
\]

As mentioned above, the time function argument \( t \) of the operator \( V^{Sys-Env}(t) \) belongs to the Dirac picture. In the Schrödinger representation, slowly time-changing terms in the interaction representation should contain rapidly time-changing exponents. These are the so-called regular time-
changing terms. In addition, there should be a part of rapidly changing terms in the interaction representation among them if the condition \( \omega \approx \omega_0 \) or any other resonance condition is not fulfilled.

It can be easily confirmed that the interaction of typical open quantum optical systems with the electromagnetic environment is described by operators that contain both rapidly time-changing and slowly time-changing terms in the interaction representation. For example,

1. for a microcavity mode coupled with a vacuum electromagnetic field at the boundary,

\[
V^{Sys-Env}(t) = \gamma_c \sum_{\omega} (c e^{-i\omega t} + c^* e^{i\omega t})(a_\omega e^{-i\omega t} + a^*_\omega e^{i\omega t}),
\]

2. for the atom and its surrounding vacuum electromagnetic field

\[
V^{Sys-Env}(t) = (d_{12} e^{-i\omega t} | e_1 > < e_2 | + d_{21} e^{i\omega t} | e_2 > < e_1 |) \int d\omega \Gamma(\omega)(a^*_\omega e^{i\omega t} + a_\omega e^{-i\omega t}).
\]

Here \( a_\omega \) and \( a^*_\omega \) are the annihilation and creation operators of bosons with the frequency \( \omega \) of a vacuum field, \( c \) and \( c^* \) are the annihilation and creation operators of bosons with the frequency \( \omega_c \) of a microcavity mode, \( | e_1 > \) and \( | e_2 > \) are the vectors of atomic quantum states with the quantum transition frequency \( \omega_0 \), \( d_{12} = d_{21}^* \) are the matrix elements of the atomic dipole moment operator; \( \Gamma(\omega) \) is the geometric form factor of a vacuum electromagnetic field. The formulas were derived by standard quantization from the expression for the energy \( V =-Ed \) of an electric dipole \( d \) in an electromagnetic field of the intensity \( E \) and energy density of an electromagnetic field \( W = \frac{1}{8\pi} (ED+BH) \) in the common region that separates the electric field of the microcavity mode from the surrounding vacuum electromagnetic field (\( D \) and \( B \) are the electric and magnetic induction, respectively, \( H \) is the intensity of magnetic field).

There arises a fundamental question of a special role of the thermal bath environment within such problems owing to the processes with different time scales in quantum optical open systems. The fact is that the time scale of the change in the operator’s rapid terms \( V^{Sys-Env}(t) \) is the revolution of the electron around the nucleus, i.e. of the order of \( 10^{-15} \) s. Further this value is to be treated as a common name regarding the fast processes related to the structure of the given objects. The formal definition of the Markov interaction process is reduced to approximating the thermal bath by the mathematical white noise with zero correlation time. This definition needs to be clarified in case of real systems where all times are finite, since along with the correlation time of the thermal bath \( \tau_{cor} \) there is a characteristic and very small scale \( 10^{-15} \) s of change in rapidly changing terms of the Hamiltonian of the open system. Understandingly, the correlation time of the thermal bath cannot be of the same order - it exceeds it \( \tau_{cor} >> 10^{-15} \) s, since in this case there is a real and sufficiently inertial process of interperticle interactions and the establishment of equilibrium inside the very thermal bath.

In the dynamics of an open system on a time scale, larger than \( 10^{-15} \) s, there are still characteristic parameters of time. These are the time of dynamic changes \( \tau_d \), the relaxation time in the Markov approximation \( \tau_{exp} \), and the total relaxation time \( \tau_\gamma \). Dynamic changes are due to exposure to an open system of coherent fields. For the environment impact to be correctly described in the Markov approximation, one can reasonably assume that \( \tau_{cor} << \tau_d \) and \( \tau_{cor} << \tau_{exp} \). In this respect, \( \tau_d >> 10^{-15} \) s, \( \tau_{exp} >> 10^{-15} \) s. In this case, before the approximation of the Markov process, it is necessary to get rid of the rapidly changing (on a scale of \( 10^{-15} \) s) terms of the initial Hamiltonian. The basis for this statement is the assumption that \( 10^{-15} s << \tau_{cor} << \tau_d, \tau_{exp}, \tau_\gamma \).

It is to be noted that the Markov approximation cannot characterize the entire range of time relaxation \( \tau_\gamma \) on time scales much larger than \( 10^{-15} \) s for the following reasons. The corresponding
Lindblad equations (1), (2) follow from the Markov approximation for various conditions of environment interaction, whence, subsequently, exponential decay laws are obtained that determine the attenuation of an open system on time scale $\tau_{\text{exp}}$. However, the spectrum of an open system is limited from below. That means that if one considers the probability $P$ that an open system was in a certain initial state $|e>$, then from the Schrödinger equation (for any system, not necessarily open with the Hamiltonian $H$ ), it is possible to derive a general expression for the probability $P = \langle e | \psi(t) | e \rangle^2$ that quantum system was in a state $|e>$:

$$P = \int_{\text{Spectrum } H} \exp(-iEt\tau^{-1})w(E)dE |^2,$$

(5)

where $|\psi(t)>$ is the wave vector of the system and its environment derived from the solution of the Schrödinger equation in the Schrödinger representation with given initial and boundary conditions, $w(E) = \sum_n C_n^2 \delta(E-E_n) + |C(E)|^2$ is the initial state spectrum $|e>$, $C_n$ and $C(E)$ are the probability amplitudes expanded in a series $|e>$ of eigen vectors $H$, related to the discrete and continuous spectrum $H$, respectively. Analytic considerations applied to formula (5) do not allow the excited state to decay exponentially over the entire time interval. On a time scale $\tau_r > \tau_{\text{exp}}$, decay should be exponential. This is determined by the analytic properties of the probability amplitude (see, Halfin’s works [4] and the review [5,6]). This stage is characterized by very rare events.

3. Global and local approaches in the theory of open systems

Regardless of the given assumption about the interconnection of various characteristic evolution times of a quantum open system, thermodynamics differentiates global and local approaches to describing dynamics of an open system. The difference between them is due both to the ways of considering the basic states, in terms of which an open system is treated, and ways of applying general methods to the initial or effective Hamiltonian of an open system and its environment.

The initial Hamiltonian of an open system and its environment $H = H^{\text{Sys}} + H^{\text{Env}} + \sqrt{V^{\text{Sys-Env}}}$ is a Hermitian Hamiltonian and thus it can be diagonalized. This procedure is quite natural for boson systems, where one can use the Bogolyubov transformation [7,8]. For other systems, diagonalization methods have also been developed, for example, using a continuous unitary transformation of the Hamiltonian and solving a nonlinear equation for the Hamiltonians [9-11]. Approaches based on such procedures for diagonalizing the initial Hamiltonian are related to the global approach within the theory of open systems. The theory also encompasses direct methods for obtaining the kinetic equation, for example, using the quantum stochastic limit, from the initial Hamiltonian [12].

Analogously, the global approach includes those ones that use the Hamiltonian diagonalization of an open system $H^{\text{Sys}}$ merely if it consists of various interacting components. In this case one can argue similar to the problem of the interaction of an atom with its environment. The Hamiltonian of electrons and the atomic nucleus interacting electromagnetically is diagonalized. The problems on the interaction of an atom with external classical electromagnetic fields, having no very strong intensities of external fields compared with intraatomic fields, have all information about an atom only in its eigenvectors $|\varepsilon_j>$ and matrix elements $d_{ij}$ of the atomic dipole moment operator. The general Hamiltonian consists of the sum of the diagonal atomic Hamiltonian and the Hamiltonian of the interaction of an atom with an external field, which is taken in the electric dipole approximation, for example, see (4).

In contrast to the processes inside a particle of an open system, for example, an atom or molecule, the interaction between particles of the very open system (molecules, impurities, quantum dots, etc.) is generally of the same order as the interaction of the particle with its environment. For example, the dipole-dipole interaction between particles of an open system occurs in the second order of the
perturbation theory when the interaction of particles (molecules or atoms) with a quantized electromagnetic field is excluded. Therefore, generally speaking, it is not very meaningful to meticulously adhere to the idea that the Hamiltonian of an open system, when neglecting interaction with the environment, should be diagonal, and therefore there arises a question to what one could attribute the dipole-dipole interaction between the components of the open system.

The role played by the initial Hamiltonian in the theory of open optical quantum systems is even more intriguing. There arose an opinion years ago that application of the initial Hamiltonian in standard procedures for obtaining the kinetic equation led to an incorrect kinetic equation that did not correspond to the dynamics of the given open system. As an example, when a quantum oscillator of a given frequency interacts with a boson thermal bath described by the interaction operator (3), the correct approach will result from discarding all rapidly time-changing terms [13], and then the interaction operator will have only the following

\[ V^{RW}(t) = \gamma_i \sum_{\omega} (c a_\omega e^{-i(\omega - \omega_i)t} + c^* a_\omega e^{i(\omega - \omega_i)t}) \]  

(6)

Such an approximation is called the rotating-wave approximation, and in addition to simple rejection, rarely does anyone consider the justification and next orders of the perturbation theory.

The use of the Hamiltonian of a rotating wave in standard procedures (for example, [14]) to obtain the kinetic equation for an open system is called the local approach to the theory of open systems. This terminology is widespread precisely among problems that use the “thermodynamic language”.

It is appropriate to recall that the initial Hamiltonian of an open quantum system and its environment is characterized by the presence of rapidly and slowly time-changing terms. Direct applying the methods of obtaining the kinetic equation does not seem to be quite correct due to the problem of the ratio of the correlation time of the thermal bath with the characteristic times of dynamics of an open system and those of changes in rapidly time-changing terms. Using the general method for deriving kinetic equations based on stochastic differential equations leads to different results depending on whether the method was applied to the initial Hamiltonian of the interaction of a two-level quantum particle with a random classical electromagnetic field in the electric dipole approximation, or whether the method was applied to the Hamiltonian of a rotating wave [15].

4. The effective Hamiltonian method

The Krylov-Bogolyubov-Mitropolsky averaging method [16, 17] is an effective method for treating various problems described by differential equations with quantities having different scales of change. This method of averaging classical differential equations has been developing since the 30s of the last century. Its participation in describing dynamics of open optical systems, functions and operators with different scales of temporal change leads to using the method of averaging rapidly changing values over the characteristic time intervals of the problem. The above-mentioned features of optical quantum systems have made it necessary to average the initial Hamiltonian of the problem

\[ H = H^{Sys} + H^{Env} + V^{Sys-Env} \]

over time intervals of the order of time \(10^{-15} s\).

As applied to optical problems involving classical fields, the Krylov-Bogolyubov-Mitropolsky method is described in the book [18], which demonstrates the effectiveness of the method while considering resonance processes of interaction of coherent optical fields with atomic-molecular systems. Works [19, 20] developed an algebraic version of the averaging method, which led to a new version of constructing the effective Hamiltonian of optical systems. The method is based on the unitary transformation of the initial Hamiltonian and the expansion of the generator of this transformation in a series in terms of the coupling constants of an open system [21]. Thus, a peculiar algebraic perturbation theory arises in this case. Works [22, 23] applied the given algebraic perturbation theory to the case of the interaction of an open system with quantized broadband fields, which led both to the development of an algorithm for dividing the environment fields into independent quantum noise sources and to the formulation of new version of constructing the effective Hamiltonian.
It should be noted that when using the Markov approximation, the diagonalization of the exact Hamiltonian of an open system and its environment is a certain excess of accuracy. It is more important to take into account the finite and long time of environment correlation in comparison with the time interval \(10^{-15} \text{s}\). Therefore, the construction of an effective Hamiltonian in the problems of the interaction of an open system with its environment is regarded as the very first step. In this context, it is important to note that the rotation wave approximation corresponds to the first order of the perturbation theory constructed on the basis of the effective Hamiltonian method.

It should be emphasized that a feature of constructing an effective Hamiltonian according to the method of [21–24] is the sequential exclusion of rapidly time-changing terms from all orders of the algebraic theory of perturbations in the interaction representation. This ensures that the condition \(10^{-15} \tau _{corr} \ll \tau _{d}, \tau _{exp}, \tau _{r}\) is satisfied upon further application of standard methods for deriving the kinetic equation (1), (2) to the obtained effective Hamiltonian. Moreover, a specific effective Hamiltonian and its corresponding Lindblad operators are obtained for each specific condition of interaction of an open system with its environment.

**Acknowledgments**

This work is supported in part by the Russian Foundation for Basic Research (grant No. 19-02-00234a).

**References**

[1] Lindblad G 1976 *Comm. Math. Phys.* **48** 119  
[2] Gorini V, Kossakowski A and Sudarshan E C G 1976 *J. Math. Phys.* **17** 821; Gorini V, Frigerio A, Verri, Kossakowski A and Sudarshan E C G 1978 *Rep. Math. Phys.* **13** 149  
[3] Holevo A 2001 *Statistical structure of quantum theory* (Berlin: Springer)  
[4] Kalfin L A 1958 *Sov. Phys. JETP* **6** 1053  
[5] Fonda L, Ghirardi G C and Rimini A 1978 *Rep. Prog. Phys.* **41** 587  
[6] Nakazato H, Namiki M and Pascazio S 1996 *Intern. J. Mod. Phys. B* **10** 247  
[7] Trushechkin A S and Volovich I V 2016 *EPL* **113** 30005  
[8] Teretenkov A E 2016 *Math. Notes* **100** 636  
[9] Wegner F 1994 *Ann. Phys.* **3** 77  
[10] Glazek S D and Wilson K G 1993 *Phys. Rev. D* **48** 5863  
[11] Glazek S D and Wilson K G 1994 *Phys. Rev. D* **49** 4214  
[12] Accardi L, Lu Y G and Volovich I 2002 *Quantum theory and its stochastic limit* (Berlin: Springer-Verlag)  
[13] Walls D F 1970 *Z. Phys.* **234** 231  
[14] Blum K. *Density Matrix Theory and Applications* (Plenum: New York, 1981).  
[15] Basharov A M 2017 *J. Phys. C. S.* **859** 012003  
[16] Krylov N M and Bogoliubov N N 1947 *Introduction to Non-Linear Mechanics* (Princeton: Princeton University Press)  
[17] Bogoliubov N and Mitropolsky Y 1961 *Asymptotic Methods in the Theory of Non-linear Oscillations* (New York: Gordon and Breach)  
[18] Butylkin V S, Kaplan A E, Khronopulo Yu G and Yakubovich E I 1989 *Resonant Nonlinear Interactions of Light with Matter* (Berlin: Springer-Verlag)  
[19] Basharov A M, Maimistov A I and Manykin E A 1983 *Sov. Phys. JETP* **57** 282  
[20] Basharov A M 1990 *Photonics. Method of unitary transformation in nonlinear optics* (in Russian, Moscow: Engineering Physics Institute)  
[21] Maimistov A I and Basharov A M 1999 *Nonlinear optical waves* (Dordrecht: Kluwer Academic)  
[22] Basharov A M 1992 *Sov. Phys. JETP* **75** 611  
[23] Basharov A M 2012 *JETP* **115** 371  
[24] Trubilko A I and Basharov A M 2020 *Phys. Scr.* **95** 045106