Kragujevac J. Sci. 47 (2025) 3 *Special Issue* 135-148 UDC 530.145:303.733.3
doi: 10.5937/KgJSci2503135A *Original scientific paper*

MARKOVIAN MASTER EQUATION FOR THREE INTERACTING QUBITS IN WEAK COUPLING LIMIT: PEDAGOGICAL EXAMPLE

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(Received November 06, 2025; Accepted November 26, 2025)

ABSTRACT. While models of one qubit and two qubits open quantum systems are widely used in contemporary physical literature, especially one dealing with the problems of quantum information and computation, model of three qubits is rarely exploited. One reason, regarding dynamics of open quantum systems, lays in the fact that adding one qubit to state space complicates considerably computational tasks. By computational tasks here is meant obtaining analytical details of dynamics, which are preferable for fundamental physical considerations. In this paper, ab initio derivation of Markovian master equation, in regime of the weak coupling limit, for three interacting qubits is presented in pedagogical manner. In this way, it will become clearer what challenges in dealing with seemingly innocuous three-qubits model are. Master equation in hand can serve for further physical inquiries, not limited to the field of quantum information and quantum computation.

Keywords: qubit, open quantum systems, Markovian dynamics

INTRODUCTION

Open quantum systems are nowadays of wide interest in both fundamental research and quantum technologies and various applications (NIELSEN and CHUANG, 2000; DEJPASAND and SASANI GHAMSARI, 2023; CHAE and CHOI, 2024). The theory of open quantum systems is still in development, with main hallmark: it is not possible to formulate canonical equation of motion, also known as quantum master equation, for open quantum system's dynamics (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). This is in sharp contrast with quantum mechanics of isolated quantum systems where Schrodinger equation governs the unitary dynamics (MESSIAH, 1962).

It turned out that it is useful to borrow concept of Markovian dynamics from classical statistical physics to single out one possible kind of dynamics of open quantum systems– quantum Markovian dynamics. Such approach is based on notion of Markovian semigroup which is related to Chapman-Kolmogorov equation of classical Markovian processes (BREUER

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and PETRUCCIONE, 2002). The result of that approach is well-known Gorini-Kossakowski-Sudarshan-Lindblad quantum master equation which is now acknowledged as one of cornerstones of open systems quantum theory (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011).

While mathematical reasoning provides the basis for rigorous proof of the existence of GKSL master equation, the physical conditions surrounding the dynamics stay secondary. Over time, mathematical physicists have developed various approaches to overcome lack of physical details, starting from microscopic picture, i.e., model Hamiltonian. One of the most prominent methods in this regard is Nakajima-Zwanzig projection technique (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). Following this route, it is possible to obtain master equation which is in GKSL form with insight into physical details at the same time.

Besides being Markovian, here we will be interested in finite-dimensional, open quantum systems, exclusively. From perspective of fundamental physics and quantum technology application, models of one and two qubits are quite well studied as a representative of finite-dimensional systems (NIELSEN and CHUANG, 2000). But realistic physical situations for sure welcome models of more than two-qubits systems, such as e.g., model of three interacting qubits as open quantum system.

So, the goal of this paper is derivation of Markovian master equation, starting from microscopic picture, for the model of three interacting qubits in contact with thermal (bosonic) bath.

This paper is structured as follows. Section *General setting* presents sketch of thinking in open quantum system theory with the aim of highlighting what is most important, starting from microscopic picture and introducing proper set of assumptions and approximations. In this way, the reader gets rough idea about what the goal is and how to reach it. Section *The model* introduces the Hamiltonian of interest revealing details which shape dynamics of open quantum system. The subsequent section, *The Algorithm*, outlines all essential computational steps in a concise form. In *Computational Details*, the procedure for obtaining the desired quantum master equation is presented. The last section is *Conclusion* of the paper. Additional details are shared in the subsequent *Appendices*.

GENERAL SETTING

Open quantum system (A) is system in unavoidable contact with another quantum system (typically with many degrees of freedom) called environment (B) (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). Basic assumption of open quantum systems theory is that A+B composite system is isolated and that dynamic of composite system is unitary. Generator of unitary dynamics is Hamiltonian of composite system:

$$H = H_A \otimes I_B + I_A \otimes H_B + \alpha H_{AB}; \tag{1}$$

H_A and H_B are self-Hamiltonians of open system and environment, respectively, while H_{AB} stands for interaction Hamiltonian which explicit form is given as

$$H_{AB} = \sum_l A_l \otimes B_l \,. \tag{2}$$

Hermitian operators A_l and B_l act on to Hilbert space of open system and environment, respectively. Coupling constant α accounts for the strength of interaction between systems A and B.

In further analysis it is convenient to introduce interaction picture with respect to the free Hamiltonian of open system and environment: $H_0 = H_A + H_B$: tilde will be used to denote operators with respect to interaction picture.

The corresponding differential form of composite system unitary dynamics is given by equation:

$$i\hbar \frac{d\tilde{\rho}_{AB}}{dt} = \left[\tilde{H}_{AB}, \tilde{\rho}_{AB}\right], \tag{3}$$

known as von Neumann-Liouville equation, where $\tilde{\rho}_{AB}$ is density operator for the whole A+B. The reduced dynamics of open system A follows by tracing out environmental degrees of freedom in Eq. (3):

$$i\hbar \frac{d\tilde{\rho}_A(t)}{dt} = tr_B\left[\tilde{H}_{AB}, \tilde{\rho}_{AB}\right], \tag{4}$$

which is starting place for further mathematical considerations (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011).

The standard approach in theory of open quantum systems consists of applying Nakajima-Zwanzig projection operator technique on Eq. (4) which leads to the following time non-local master equation (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011):

$$\frac{d\tilde{\rho}_A(t)}{dt} = \int_{t_0}^{t} \mathcal{K}(t-s)\, \tilde{\rho}_A(s)ds,\ \ \tilde{\rho}_A(t_0) = \rho_{A0}\ , \tag{5}$$

where $\mathcal{K}(t)$ is so called memory kernel which tells how the change of $\tilde{\rho}_A(t)$ depends on its history. In other words, dynamic of open quantum system is non-Markovian. Eq. (5) is, from mathematical point of view, intractable if proper assumptions and approximations are not invoked. For the sake of completeness, it is important to note that it is possible (and desirable) to describe quantum non-Markovian processes through local in time master equation (via technique of time-convolutionless forms or TCL for short (BREUER and PETRUCCIONE, 2002) which is perfectly equivalent to results obtained by Nakajima-Zwanzig technique (CHRUŚCIŃSKI and KOSSAKOWSKI, 2012). General form of this TCL master equation is given by:

$$\frac{d\tilde{\rho}_A(t)}{dt} = \mathcal{L}(t-t_0)\tilde{\rho}_A(t), \tilde{\rho}_A(t_0) = \rho_{A0}, \tag{6}$$

where $\mathcal{L}$ is superoperator known as (time dependent) Liouvillian of master equation.

The question(s) of open system's non-Markovianity quantification and description is tightly connected with the notion of quantum Markovianity (BREUER, 2012). Quantum Markovianity of open system dynamics is reflected in the fact that corresponding dynamical map fulfill semigroup and divisibility property. Divisibility property is analogous to Chapman-Kolmogorov equation which defines the notion of classical Markovianity (BREUER and PETRUCCIONE, 2002).

By dynamical map here is meant mapping $\Lambda(t, t_0)$:

$$\rho(t) = \Lambda(t, t_0)\rho(t_0) \tag{7}$$

i.e. integral form of dynamical law. In other words, $\Lambda(\mathrm{t}, \mathrm{t}_0)$ for Markovian dynamics satisfies equation

$$\frac{d\Lambda(t,t_0)}{dt} = \mathcal{L}_M \Lambda(t,t_0), \Lambda(t_0,t_0) = \mathbb{I}, \tag{8}$$

whose solution is given by:

$$\Lambda(t,t_0) = e^{(t-t_0)\mathcal{L}_M}, \tag{9}$$

where $\mathcal{L}_M$ is generator of the semigroup and M stand for Markovian. Eq. (9) implies that $\Lambda(t,t_0)$ depends only upon the difference "$t - t_0$" and hence $\Lambda(t) \equiv \Lambda(t,0)$ defines one-parameter semigroup satisfying composition law

$$\Lambda(t_1)\Lambda(t_2) = \Lambda(t_1 + t_2), \tag{10}$$

which is an instance of map divisibility (BREUER, 2012).

Requests for quantum Markovian (in above sense) and completely positive and trace-preserving (CPTP) dynamics led to mathematical derivation of master equation in the well-known form (RIVAS and HUELGA, 2011):

$$\frac{d\tilde{\rho}_A(t)}{dt} = -\frac{i}{\hbar}[H_{LS}, \tilde{\rho}_A] + \sum_k \gamma_k \left(V_k \tilde{\rho}_A V_k^\dagger - \frac{1}{2}\{V_k^\dagger V_k, \tilde{\rho}_A\}\right) = \mathcal{L}_M \tilde{\rho}_A,\ \tilde{\rho}_A(t_0) = \rho_0 \tag{11}$$

which is due to Gorini, Kosakowski, Sudarshan and Lindblad (GKSL). $\gamma_k's$ are decay rates, V_k are Lindblad operators while H_{LS} stands for so called Lamb shift which produces a shift in the energy levels of the open quantum system. $\mathcal{L}_M$, in the context of Eq. (11) is also called Liovillian of master equation. $\{A, B\} = AB + BA$ is standard notation for anticommutator of two operators.

It is known that Liouvillian of Eq. (11) generalizes to (not to be confused with Eq. (6)) (RIVAS and HUELGA, 2011)

$$\mathcal{L}_M(t)\tilde{\rho}_A = -\frac{i}{\hbar}[H(t), \tilde{\rho}_A] + \sum_k \gamma_k(t) \left(V_k(t)\tilde{\rho}_A V_k^\dagger(t) - \frac{1}{2}\{V_k^\dagger(t)V_k(t), \tilde{\rho}_A\}\right), \tag{12}$$

where symbols have the same meaning as in Eq. (11), only now time dependent. Interestingly, Eq. (12) accounts for non-Markovian dynamics if $\gamma_k(t) < 0$, for at least one k. Because of the last feature, Eq. (11) will be of only interest for further considerations.

We will not dwell here on the problems which surround quantification or rigorous definition of quantum Markovianity, question which is not settled, in unambiguous manner, yet (BREUER, 2012). In other words, in this paper, property expressed by Eq. (10) is basic for definition of quantum Markovianity. But it should be kept in mind that it is not the only point of view in contemporary literature, i.e. Eq. (10) is not considered sufficient condition (RIVAS and HUELGA, 2011).

Rather, we would like to emphasize that situations where dynamics is Markovian (in sense of Eq. (11) i.e. Eq. (10)) still offer rich physics from the perspective of fundamentals and applications. In other words, basic quantum phenomena such as quantum dissipation, quantum decay and quantum decoherence (JOOS *et al.*, 2003, SCHLOSSHAUER, 2007, GARDINER and ZOLLER, 2004) can be modeled and studied in framework of Markovianity expressed by Eq. (11). From computational point of view, despite unsettled definition, Markovian dynamics is easier to handle.

At this point, a brief remark is in order. As will be seen, different notations will be used for frequencies. To avoid possible confusion, let us emphasize that ω will be used for the frequencies (and frequency differences) of the open system and will always be a discrete quantity. On the other hand, Ω will be used to denote the frequencies of the environment and may represent either a discrete (as in Eq. (18)) or a continuous (as in Eq. (29)) quantity.

THE MODEL

As open, quantum finite-dimensional system (A) of interest here it will be considered system of three mutually interacting qubits that interact with infinite-dimensional thermal bath of harmonic oscillators, i.e., environment (B).

The free Hamiltonians, cf. Eq. (1), of open quantum system and bosonic bath are $H_A = \omega_0(S_{1z} + S_{2z} + S_{3z}) + \beta S_{1z} \otimes S_{2z} \otimes I_3$ and $H_B = \sum_{\vec{k}} \hbar\Omega_{\vec{k}} b_{\vec{k}}^\dagger b_{\vec{k}}$, respectively. β plays role of intercoupling constant whereby it is assumed that $\beta > \alpha$. Interaction part of Hamiltonian, $H_{AB} = (S_{1x} + S_{2x} + S_{3x}) \otimes \sum_{\vec{k}} g_{\vec{k}} \left(b_{\vec{k}}^\dagger + b_{\vec{k}}\right) \equiv A \otimes B$, stands for interaction between open system and environment with $g_{\vec{k}}$ playing the role of coupling constant α. Operators S_{iz} and S_{ix} are standard spin-1/2 operators, while bosonic operators $b_{\vec{k}}^\dagger$ and $b_{\vec{k}}$ fulfil commutation relations $\left[b_{\vec{k}}, b_{\vec{k}'}^\dagger\right] = \delta_{\vec{k}\vec{k}'}$ (MESSIAH, 1962).

By thermal bath here is meant multimode bosonic environment which separable state is given by reduced density operator (BREUER and PETRUCCIONE, 2002):

$$\rho_B = \prod_{\vec{k}} \left[1 - e^{-\frac{\hbar\Omega_{\vec{k}}}{k_B T}}\right] e^{-\frac{\hbar\Omega_{\vec{k}} b_{\vec{k}}^\dagger b_{\vec{k}}}{k_B T}}, \tag{13}$$

where k_B is Boltzmann constant and T is temperature of the bath. Multimode character is expressed by frequency $\Omega_{\vec{k}}$ where $\vec{k}$ is wave vector taking discrete values. It will turn out that thermal averages of bosonic operators are needed, so for convenience they are listed here:

$$\langle b_{\vec{k}}^\dagger \rangle = \langle b_{\vec{k}} \rangle = 0, \tag{14a}$$

$$\langle b_{\vec{k}} b_{\vec{k}'} \rangle = \langle b_{\vec{k}}^\dagger b_{\vec{k}'}^\dagger \rangle = 0, \tag{14b}$$

$$\langle b_{\vec{k}}^\dagger b_{\vec{k}'} \rangle = \langle n_{\vec{k}} \rangle \, \delta_{\vec{k}\vec{k}'}, \tag{14c}$$

$$\langle b_{\vec{k}} b_{\vec{k}'}^\dagger \rangle = \left(1 + \langle n_{\vec{k}} \rangle\right) \delta_{\vec{k}\vec{k}'}, \tag{14d}$$

where $\langle n_{\vec{k}} \rangle = \frac{1}{e^{\frac{\hbar\Omega_{\vec{k}}}{k_B T}} - 1}$ stands for thermal average number of bosons in a mode with frequency $\Omega_{\vec{k}}$. Some details concerning averages, Eqs. (14), can be found in Appendix 2.

THE ALGORITHM

Mathematical derivation of Eq. (11) does not say much about the microscopic origin of dynamics and physical limitations of GKSL master equation. To continue further, it is necessary to characterize properties of the environment and strength of the interaction between systems A and B, to begin with. Then using technique of Nakajima-Zwanzig and invoking famous set of approximations–Born, Markov and secular–it is possible to obtain GKSL form of master equation. Interested reader may find appropriate details related to microscopic derivation of GKSL master equation in (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011): for purposes of this paper, we will use only some points of immediate interest.

Following this route of obtaining GKSL master equation it turns out that Eq. (11) can be formulated in the following, unitarily equivalent, form:

$$\frac{d\tilde{\rho}_A}{dt} = -\frac{i}{\hbar}[H_{LS}, \tilde{\rho}_A] + \sum_{\omega}\sum_{kl}\gamma_{kl}(\omega)\left(A_l(\omega)\tilde{\rho}_A A_k^{\dagger}(\omega) - \frac{1}{2}\{A_k^{\dagger}(\omega)A_l(\omega), \tilde{\rho}_A\}\right). \quad (15)$$

In Eq. (15), $\gamma_{kl}(\omega)$ are matrix elements of positive semidefinite matrix, for all ω, which may be diagonalized by unitary matrix, where elements on diagonal are decay rates from Eq. (11). Using matrix elements, u_{ki}, from unitary transformation, we may write relation $A_i = \sum_{k=1}^{d^2-1} u_{ki} V_k$ between new (A_i) and old (V_k) Lindblad operators, where d stands for dimensionality of open system' Hilbert space. Unitary equivalence means that Eq. (11) and Eq. (15) describe the same dynamics. So, we will refer to Eq. (15) further on.

To be able to write down master equation, Eq. (15), it is necessary to find operators $A_l(\omega)$ and H_{LS} as well as the functions $\gamma_{kl}(\omega)$.

The expressions for $A_l(\omega)$ are obtained by taking interaction part of Hamiltonian, H_{AB}, in interaction picture:

$$\tilde{H}_{AB} = U_0^{\dagger}(\sum_l A_l \otimes B_l)U_0 = \sum_l \tilde{A}_l(t) \otimes \tilde{B}_l(t)\,; \quad (16)$$

$U_0 = U_A \otimes U_B$ stands for unitary operator having in mind standard quantum-mechanics equality $U_m = e^{-\frac{i}{\hbar}tH_m}$ where $m = A, B$. Writing Eq. (16) in explicit form leads to the expression $\tilde{H}_{AB} = \sum_l \sum_{\omega} A_l(\omega)\, e^{-i\omega t} \otimes \sum_{\Omega_m} B_l(\Omega)\, e^{-i\Omega_m t}$ with operators:

$$A_l(\omega) = \sum_{\varepsilon_A - \varepsilon_A' = \hbar\omega} |\varepsilon_A\rangle\langle\varepsilon_A|A_l|\varepsilon_A'\rangle\langle\varepsilon_A'| \quad (17)$$

and

$$B_l(\Omega_m) = \sum_{\varepsilon_B - \varepsilon_B' = \hbar\Omega_m} |\varepsilon_B\rangle\langle\varepsilon_B|B_l|\varepsilon_B'\rangle\langle\varepsilon_B'|. \quad (18)$$

In Eqs. (17) and (18) ω and Ω represent open system and environment frequencies, respectively, while ε_A is running through the discrete spectrum of H_A and ε_B is running through the discrete spectrum of H_B. Operators $A_l(\omega)$ from Eq. (17) are just those from Eq. (15), so Eq. (17) can be considered as defining equation.

The properties of the environment are encapsulated in Fourier transformation of correlation functions which is defined as $\langle\tilde{B}_k^{\dagger}(t)\tilde{B}_l(t-s)\rangle = tr[\tilde{B}_k^{\dagger}(t)\tilde{B}_l(t-s)\rho_B]$, in general (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). If the state of the environment is stationary (here thermodynamic equilibrium) and equation $[H_B, \rho_B] = 0$ holds, then previous equality simplifies $\langle\tilde{B}_k^{\dagger}(t)\tilde{B}_l(0)\rangle = tr[\tilde{B}_k^{\dagger}(t)B_l\rho_B]$. The one-sided Fourier transformation of the correlation functions in this case reads:

$$\Gamma_{kl}(\omega) = \int_0^{+\infty} dt e^{i\omega t}\, tr[\tilde{B}_k^{\dagger}(t)B_l\rho_B]. \quad (19)$$

It is convenient to decompose Eq. (19) as follows:

$$\Gamma_{kl}(\omega) = \frac{1}{2}\gamma_{kl}(\omega) + iS_{kl}(\omega). \quad (19a)$$

For the stationary state (e.g. Eq. (13)) of the environment, functions $\gamma_{kl}(\omega)$ are defined by the following equality in interaction picture:

$$\gamma_{kl}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t}\, tr[\tilde{B}_k^{\dagger}(t)B_l\rho_B],$$

while defining equation for Lamb-shift Hamiltonian, H_{LS}, reads (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011):

$$H_{LS} = \sum_{\omega} \sum_{k,l} S_{kl}(\omega) A_k^{\dagger}(\omega) A_l(\omega);$$

so having expressions for $\Gamma_{kl}(\omega)$ and $\gamma_{kl}(\omega)$ automatically yields an expression for $S_{kl}(\omega)$.

For the present model, an interaction Hamiltonian of the form $H_{AB} = A \otimes B$ results in simplified expressions for the decay rates and the Lamb shift:

$$\gamma(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t}\, tr[\tilde{B}(t) B \rho_B], \quad (20)$$

and

$$H_{LS} = \sum_{\omega} S(\omega)\, A^{\dagger}(\omega) A(\omega), \quad (21)$$

which will be of immediate interest further on.

COMPUTATIONAL DETAILS

The first step is solving eigenvalue problem of open system Hamiltonian H_A, i.e. $H_A|\epsilon_i\rangle = \epsilon_i|\epsilon_i\rangle$. It is not hard to check that set of eigenvalues and eigenvectors are those given in Table 1, whence it is noted that eigenvectors are tensor product of eigenstates of the S_z operator, $|g\rangle$ and $|e\rangle$.

From general expression $A(\omega) = \sum_{\omega=\varepsilon_j-\varepsilon_i} |\varepsilon_i\rangle\langle\varepsilon_i|A|\varepsilon_j\rangle\langle\varepsilon_j|$ follows that it is necessary to write down all differences of eigenvalues $\varepsilon_j - \varepsilon_i$. To be more tractable those data are presented in Table 2.

Table 1 Eigenvalues and eigenvectors of open system's Hamiltonian.

Eigenvalues	Eigenvectors
$\epsilon_1 = \frac{\beta}{4} - \frac{3\omega_0}{2}$	$\lvert\epsilon_1\rangle = \lvert g\rangle\lvert g\rangle\lvert g\rangle$
$\epsilon_2 = \frac{\beta}{4} - \frac{\omega_0}{2}$	$\lvert\epsilon_2\rangle = \lvert g\rangle\lvert g\rangle\lvert e\rangle$
$\epsilon_3 = -\frac{\beta}{4} - \frac{\omega_0}{2}$	$\lvert\epsilon_3\rangle = \lvert g\rangle\lvert e\rangle\lvert g\rangle$
$\epsilon_4 = \frac{\beta}{4} + \frac{\omega_0}{2}$	$\lvert\epsilon_4\rangle = \lvert g\rangle\lvert e\rangle\lvert e\rangle$
$\epsilon_5 = -\frac{\beta}{4} - \frac{\omega_0}{2}$	$\lvert\epsilon_5\rangle = \lvert e\rangle\lvert g\rangle\lvert g\rangle$
$\epsilon_6 = -\frac{\beta}{4} + \frac{\omega_0}{2}$	$\lvert\epsilon_6\rangle = \lvert e\rangle\lvert g\rangle\lvert e\rangle$
$\epsilon_7 = \frac{\beta}{4} + \frac{\omega_0}{2}$	$\lvert\epsilon_7\rangle = \lvert e\rangle\lvert e\rangle\lvert g\rangle$
$\epsilon_8 = \frac{\beta}{4} + \frac{3\omega_0}{2}$	$\lvert\epsilon_8\rangle = \lvert e\rangle\lvert e\rangle\lvert e\rangle$

A closer look at Table 2 shows that there are mutually equal differences $\varepsilon_j - \varepsilon_i$. For example,
$\varepsilon_1 - \varepsilon_2 = -\omega_0$, $\varepsilon_2 - \varepsilon_7 = -\omega_0$, $\varepsilon_3 - \varepsilon_4 = -\omega_0$, $\varepsilon_3 - \varepsilon_6 = -\omega_0$, $\varepsilon_5 - \varepsilon_4 = -\omega_0$, $\varepsilon_5 - \varepsilon_6 = -\omega_0$, $\varepsilon_7 - \varepsilon_8 = -\omega_0$. For this particular frequency, $-\omega_0$, Eq. (17) takes the form:
$A(-\omega_0) = |\varepsilon_2\rangle\langle\varepsilon_2|A|\varepsilon_1\rangle\langle\varepsilon_1| + |\varepsilon_7\rangle\langle\varepsilon_7|A|\varepsilon_2\rangle\langle\varepsilon_2| + |\varepsilon_4\rangle\langle\varepsilon_4|A|\varepsilon_3\rangle\langle\varepsilon_3| + |\varepsilon_6\rangle\langle\varepsilon_6|A|\varepsilon_3\rangle\langle\varepsilon_3| +$
$+|\varepsilon_4\rangle\langle\varepsilon_4|A|\varepsilon_5\rangle\langle\varepsilon_5| + |\varepsilon_6\rangle\langle\varepsilon_6|A|\varepsilon_5\rangle\langle\varepsilon_5| + |\varepsilon_8\rangle\langle\varepsilon_8|A|\varepsilon_7\rangle\langle\varepsilon_7|$,
bearing in mind that $A = S_{1x} + S_{2x} + S_{3x}$.

All in all, following the Table 2 becomes clear that it is needed to find the following operators: $A(0)$, $A(\pm\omega_0)$, $A(\pm 2\omega_0)$, $A(\pm 3\omega_0)$, $A\left(\pm\frac{\beta}{2}\right)$, $A\left(\pm\frac{\beta-2\omega_0}{2}\right)$, $A\left(\pm\frac{\beta+2\omega_0}{2}\right)$, $A\left(\pm\frac{\beta-4\omega_0}{2}\right)$ and $A\left(\pm\frac{\beta+4\omega_0}{2}\right)$. Having in mind relation $[A(-\omega)]^\dagger = A(\omega)$, it is enough to calculate frequencies with negative signs. With the help of expressions for spin operators (see Appendix 1), after some algebra, follows that non-zero contributions come from operators $A(\pm\omega_0)$, $A\left(\pm\frac{\beta-2\omega_0}{2}\right)$ and $A\left(\pm\frac{\beta+2\omega_0}{2}\right)$, i.e.:

$$A(\pm\omega_0) = I_1 \otimes I_2 \otimes \tfrac{1}{2} S_{3\mp},$$
$$A\left(\pm\tfrac{\beta-2\omega_0}{2}\right) = \tfrac{1}{2} S_{1\pm} \otimes \tfrac{1}{2}(I_2 + 2S_{2z}) \otimes I_3 + \tfrac{1}{2}(I_1 + 2S_{1z}) \otimes \tfrac{1}{2} S_{2\pm} \otimes I_3,$$
$$A\left(\pm\tfrac{\beta+2\omega_0}{2}\right) = \tfrac{1}{2} S_{1\mp} \otimes \tfrac{1}{2}(I_2 - 2S_{2z}) \otimes I_3 + \tfrac{1}{2}(I_1 - 2S_{1z}) \otimes \tfrac{1}{2} S_{2\mp} \otimes I_3. \quad (22)$$

Table 2 Eigenvalue differences.

$\varepsilon_1 - \varepsilon_2 = -\omega_0$	$\varepsilon_2 - \varepsilon_1 = \omega_0$	$\varepsilon_3 - \varepsilon_1 = \omega_0 - \frac{\beta}{2}$	$\varepsilon_4 - \varepsilon_1 = -\frac{\beta-4\omega_0}{2}$
$\varepsilon_1 - \varepsilon_3 = \frac{\beta-2\omega_0}{2}$	$\varepsilon_2 - \varepsilon_3 = \frac{\beta}{2}$	$\varepsilon_3 - \varepsilon_2 = -\frac{\beta}{2}$	$\varepsilon_4 - \varepsilon_2 = -\frac{\beta-2\omega_0}{2}$
$\varepsilon_1 - \varepsilon_4 = \frac{\beta-4\omega_0}{2}$	$\varepsilon_2 - \varepsilon_4 = \frac{\beta-2\omega_0}{2}$	$\varepsilon_3 - \varepsilon_4 = -\omega_0$	$\varepsilon_4 - \varepsilon_3 = \omega_0$
$\varepsilon_1 - \varepsilon_5 = \frac{\beta-2\omega_0}{2}$	$\varepsilon_2 - \varepsilon_5 = \frac{\beta}{2}$	$\varepsilon_3 - \varepsilon_5 = 0$	$\varepsilon_4 - \varepsilon_5 = \omega_0$
$\varepsilon_1 - \varepsilon_6 = \frac{\beta-4\omega_0}{2}$	$\varepsilon_2 - \varepsilon_6 = \frac{\beta-2\omega_0}{2}$	$\varepsilon_3 - \varepsilon_6 = -\omega_0$	$\varepsilon_4 - \varepsilon_6 = 0$
$\varepsilon_1 - \varepsilon_7 = -2\omega_0$	$\varepsilon_2 - \varepsilon_7 = -\omega_0$	$\varepsilon_3 - \varepsilon_7 = -\frac{\beta+2\omega_0}{2}$	$\varepsilon_4 - \varepsilon_7 = -\frac{\beta}{2}$
$\varepsilon_1 - \varepsilon_8 = -3\omega_0$	$\varepsilon_2 - \varepsilon_8 = -2\omega_0$	$\varepsilon_3 - \varepsilon_8 = -\frac{\beta+4\omega_0}{2}$	$\varepsilon_4 - \varepsilon_8 = -\frac{\beta+2\omega_0}{2}$
$\varepsilon_5 - \varepsilon_1 = -\frac{\beta+2\omega_0}{2}$	$\varepsilon_6 - \varepsilon_1 = -\frac{\beta-4\omega_0}{2}$	$\varepsilon_7 - \varepsilon_1 = 2\omega_0$	$\varepsilon_8 - \varepsilon_1 = 3\omega_0$
$\varepsilon_5 - \varepsilon_2 = -\frac{\beta}{2}$	$\varepsilon_6 - \varepsilon_2 = -\frac{\beta-2\omega_0}{2}$	$\varepsilon_7 - \varepsilon_2 = \omega_0$	$\varepsilon_8 - \varepsilon_2 = 2\omega_0$
$\varepsilon_5 - \varepsilon_3 = 0$	$\varepsilon_6 - \varepsilon_3 = \omega_0$	$\varepsilon_7 - \varepsilon_3 = \frac{\beta+2\omega_0}{2}$	$\varepsilon_8 - \varepsilon_3 = \frac{\beta+4\omega_0}{2}$
$\varepsilon_5 - \varepsilon_4 = -\omega_0$	$\varepsilon_6 - \varepsilon_4 = 0$	$\varepsilon_7 - \varepsilon_4 = \frac{\beta}{2}$	$\varepsilon_8 - \varepsilon_4 = \frac{\beta+2\omega_0}{2}$
$\varepsilon_5 - \varepsilon_6 = -\omega_0$	$\varepsilon_6 - \varepsilon_5 = \omega_0$	$\varepsilon_7 - \varepsilon_5 = \frac{\beta+2\omega_0}{2}$	$\varepsilon_8 - \varepsilon_5 = \frac{\beta+4\omega_0}{2}$
$\varepsilon_5 - \varepsilon_7 = -\frac{\beta+2\omega_0}{2}$	$\varepsilon_6 - \varepsilon_7 = -\frac{\beta}{2}$	$\varepsilon_7 - \varepsilon_6 = \frac{\beta}{2}$	$\varepsilon_8 - \varepsilon_6 = \frac{\beta+2\omega_0}{2}$
$\varepsilon_5 - \varepsilon_8 = -\frac{\beta+4\omega_0}{2}$	$\varepsilon_6 - \varepsilon_8 = -\frac{\beta+2\omega_0}{2}$	$\varepsilon_7 - \varepsilon_8 = -\omega_0$	$\varepsilon_8 - \varepsilon_7 = \omega_0$

Having Eqs. (22), next to be calculated is function $\Gamma(\omega)$. The environment degrees of freedom in interaction Hamiltonian are represented by operator $B = \sum_{\vec{k}} g_{\vec{k}} \left(b_{\vec{k}}^\dagger + b_{\vec{k}}\right)$ which in interaction picture takes the form $\tilde{B}(t) = \sum_{\vec{k}} g_{\vec{k}} \left(b_{\vec{k}}^\dagger e^{i t \Omega_k} + b_{\vec{k}} e^{-i t \Omega_k}\right)$. Putting these two into $\Gamma(\omega) = \int_0^{+\infty} dt e^{i\omega t}\, tr[\tilde{B}(t) B \rho_B]$ and making use of Eqs. (14) follows:

$$\Gamma(\omega) = \sum_{\vec{k}} \int_0^{+\infty} dt\; g_{\vec{k}}^2 \langle n_{\vec{k}} \rangle e^{it(\omega+\Omega_k)} + \sum_{\vec{k}} \int_0^{+\infty} dt\; g_{\vec{k}}^2 (1 + \langle n_{\vec{k}} \rangle) e^{it(\omega-\Omega_k)}. \quad (23)$$

Similarly, the expression for decay rate function read:

$$\gamma(\omega)=\sum_{\vec{k}}\int_{-\infty}^{+\infty}dt\ \ g_{\vec{k}}^{2}\langle n_{\vec{k}}\rangle\, e^{it(\omega+\Omega_k)}\ +\sum_{\vec{k}}\int_{-\infty}^{+\infty}dt\ \ g_{\vec{k}}^{2}(1+\langle n_{\vec{k}}\rangle)e^{it(\omega-\Omega_k)}. \quad (24)$$

Integrals $\int_0^{+\infty}dt\, e^{it(\omega\pm\Omega_k)}$ and $\int_{-\infty}^{+\infty}dt\, e^{it(\omega\pm\Omega_k)}$ are not well-defined in sense of improper Riemann integrals, but do make sense in distribution theory–for details see (RIVAS and HUELGA, 2011) and references therein. Here, we are interested in final forms of those integrals, which read:

$$\int_0^{+\infty}dt\, e^{it(\omega\pm\Omega_k)}=\frac{i}{\omega\pm\Omega_k}+\pi\delta(\omega\pm\Omega_k)$$

and

$$\int_{-\infty}^{+\infty}dt\, e^{it(\omega\pm\Omega_k)}=2\pi\delta(\omega\pm\Omega_k),$$

where δ denotes Dirac delta function.

Making use of these integrals, Eqs. (23) and (24) transform into expressions:

$$\Gamma(\omega)=\sum_{\vec{k}}g_{\vec{k}}^{2}\langle n_{\vec{k}}\rangle\left(\frac{i}{\omega+\Omega_k}+\pi\delta(\omega+\Omega_k)\right)+\sum_{\vec{k}}g_{\vec{k}}^{2}\left(1+\langle n_{\vec{k}}\rangle\right)\left(\frac{i}{\omega-\Omega_k}+\pi\delta(\omega-\Omega_k)\right) \quad (25)$$

and

$$\gamma(\omega)=2\pi\sum_{\vec{k}}g_{\vec{k}}^{2}\langle n_{\vec{k}}\rangle\,\delta(\omega+\Omega_k)\ +2\pi\sum_{\vec{k}}g_{\vec{k}}^{2}(1+\langle n_{\vec{k}}\rangle)\delta(\omega-\Omega_k), \quad (26)$$

respectively. Comparing last two expressions with Eq. (19a) follows equation for $S(\omega)$:

$$S(\omega)=\sum_{\vec{k}}g_{\vec{k}}^{2}\left(\frac{\langle n_{\vec{k}}\rangle}{\omega+\Omega_k}+\frac{1+\langle n_{\vec{k}}\rangle}{\omega-\Omega_k}\right). \quad (27)$$

At this point it is convenient to switch from sums over modes in Eqs. (25) and (26) to integrals. Justification for doing this comes from two reasons. First reason is of formal nature: it is easier mathematically to handle integrals than sums. The second reason is physical: the bath has vast degrees of freedom making the spectrum of H_B practically continuous. Eqs. (26) and (27) now read:

$$\gamma(\omega)=\int_0^{\infty}d\Omega\, J(\Omega)\langle n(\Omega)\rangle\delta(\omega+\Omega)+\int_0^{\infty}d\Omega\, J(\Omega)(1+\langle n(\Omega)\rangle)\delta(\omega-\Omega),\ \text{i.e.}$$

$$\gamma(\omega)=\begin{cases}J(|\omega|)\langle n(|\omega|)\rangle, & \omega<0\\ J(|\omega|)(1+\langle n(|\omega|)\rangle), & \omega\geq 0\end{cases} \quad (28)$$

and

$$S(\omega)=\int_0^{\infty}d\Omega\, J(\Omega)\left(\frac{\langle n(\Omega)\rangle}{\omega+\Omega}+\frac{1+\langle n(\Omega)\rangle}{\omega-\Omega}\right). \quad (29)$$

In the context of a bosonic bath, negative frequencies correspond to the physical process of the system absorbing energy from the bath, while positive frequencies describe the system emitting energy into the bath. Here, $J(\Omega)$ is the so-called spectral density of the bath and contains information about the strength of coupling per frequency. Basically, $J(\Omega)$ occurs by smoothing $g_{\vec{k}}^{2}$. Just as an example, the so-called ohmic spectral density is given by the equation:

$$J(\Omega)=2\pi\sum_{\vec{k}}g_{\vec{k}}^{2}\delta(\Omega-\Omega_k)\xrightarrow{yields}J(\Omega)=2\pi\alpha\Omega e^{-\Omega/\Omega_c} \quad (30)$$

where α is a constant that modifies strength of interaction and Ω_c is cut-off frequency (RIVAS *et al.*, 2010). Spectral density, Eq. (29), is well suited for Markovian dynamics, especially for the bath at high temperatures. Nevertheless, other choices of spectral densities can be made but with the caveat that the validity of the master equation itself may be brought into question. We will not pursue further questions about explicit form and properties of spectral density: these questions are important when it comes to analysis of dynamics governed by master equation, whether numerically or analytically.

Using formula Eq. (21) and operators Eqs. (22) it is possible to show (by simple, but tedious algebra) that expression for Lamb shift takes the form:

$H_{LS} = \sum_{i=1}^{7} c_i G_i,$

where

$$c_1 = \frac{\hbar^2(3S(\omega_0)+\hbar^2 S(\omega_0)-2\mathbb{I}\omega_0)}{2\sqrt{2}},\ c_2 = \frac{2\mathbb{I}\hbar^2\omega_0}{\sqrt{2}},\ c_3 = \frac{\hbar^2((1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}},$$
$$c_4 = \frac{\hbar^2((1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}},\ c_5 = \frac{-2\hbar^3(\mathbb{I}\beta+S(\omega_0)-2\mathbb{I}\omega_0)}{\sqrt{2}},\ c_6 = \frac{\hbar^2(2\mathbb{I}\beta\hbar+(1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}},$$
$$c_7 = \frac{\hbar^2(2\mathbb{I}\beta\hbar+(1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}} \tag{31}$$

and

$$G_1 = \frac{1}{2\sqrt{2}} I_1 \otimes I_2 \otimes I_3,\ G_2 = \frac{2}{\hbar} I_1 \otimes I_2 \otimes S_{3z},\ G_3 = \frac{2}{\hbar} I_1 \otimes S_{2z} \otimes I_3,\ G_4 = \frac{2}{\hbar} S_{1z} \otimes I_2 \otimes I_3,$$
$$G_5 = \frac{\sqrt{2}}{\hbar^2} S_{1z} \otimes S_{2z} \otimes I_3,\ G_6 = \frac{\sqrt{2}}{\hbar^2} S_{1x} \otimes S_{2x} \otimes I_3,\ G_7 = \frac{\sqrt{2}}{\hbar^2} S_{1y} \otimes S_{2y} \otimes I_3. \tag{32}$$

In above expressions, $S(\omega_0)$ is defined by Eq. (29), $\mathbb{I} = \int_0^\infty d\Omega\, J(\Omega) \frac{\omega(1+2\langle n(\Omega)\rangle)+\Omega}{\omega^2 - \Omega^2}$ and β is intercoupling constant introduced in *The model* section.

The desired master equation for three qubits immersed in thermal, bosonic bath takes the simplified form:

$$\frac{d\tilde{\rho}_A}{dt} = -\frac{i}{\hbar}[H_{LS}, \tilde{\rho}_A] + \sum_\omega \gamma(\omega)\left(A(\omega)\tilde{\rho}_A A^\dagger(\omega) - \frac{1}{2}\{A^\dagger(\omega)A(\omega), \tilde{\rho}_A\}\right), \tag{33}$$

where ω runs through allowed positive and negative frequencies.

In the literature, it is common for master equations concerning qubit systems to be expressed in terms of Pauli operators, $\vec{\sigma}$, bearing in mind that $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$. Therefore, the final form of the master equation will also be written in this way here, considering the identity $\sigma_\pm\sigma_\mp = 2(1 \mp \sigma_z)$. Clearly, it is understood that the Lamb shift is also expressed in terms of Pauli operators. So, interaction-picture quantum Markovian master equation reads:

$$\frac{d\tilde{\rho}_A}{dt} = -\frac{i}{\hbar}[H_{LS}, \tilde{\rho}_A] + \frac{\boldsymbol{\gamma(\omega_0)}}{\mathbf{16}}\left(I_1 \otimes I_2 \otimes \sigma_{3-} \tilde{\rho}_A I_1 \otimes I_2 \otimes \sigma_{3+} - \frac{1}{2}\{I_1 \otimes I_2 \otimes \sigma_{3+}\sigma_{3-}, \tilde{\rho}_A\}\right)$$
$$+ \frac{\boldsymbol{\gamma(-\omega_0)}}{\mathbf{16}}\left(I_1 \otimes I_2 \otimes \sigma_{3+} \tilde{\rho}_A I_1 \otimes I_2 \otimes \sigma_{3-} - \frac{1}{2}\{I_1 \otimes I_2 \otimes \sigma_{3-}\sigma_{3+}, \tilde{\rho}_A\}\right)$$
$$+ \frac{\boldsymbol{\gamma\left(\frac{\beta - 2\omega_0}{2}\right)}}{\mathbf{64}}\left(\left(\sigma_{1+} \otimes \frac{\sigma_{2-}\sigma_{2+}}{2} \otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2} \otimes \sigma_{2+} \otimes I_3\right)\tilde{\rho}_A\left(\sigma_{1-} \otimes \frac{\sigma_{2-}\sigma_{2+}}{2} \otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2} \otimes \sigma_{2-} \otimes I_3\right)\right.$$
$$\left. - \frac{1}{2}\left\{\left(\sigma_{1-} \otimes \frac{\sigma_{2-}\sigma_{2+}}{2} \otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2} \otimes \sigma_{2-} \otimes I_3\right)\left(\sigma_{1+} \otimes \frac{\sigma_{2-}\sigma_{2+}}{2} \otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2} \otimes \sigma_{2+} \otimes I_3\right), \tilde{\rho}_A\right\}\right)$$

$$+\frac{\gamma\left(-\frac{\boldsymbol{\beta}-2\boldsymbol{\omega_0}}{2}\right)}{\mathbf{64}}\left(\left(\sigma_{1-}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2-}\otimes I_3\right)\tilde{\rho}_A\left(\sigma_{1+}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2+}\otimes I_3\right)\right.$$
$$\left.-\frac{1}{2}\left\{\left(\sigma_{1+}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2+}\otimes I_3\right)\left(\sigma_{1-}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2-}\otimes I_3\right),\tilde{\rho}_A\right\}\right)$$
$$+\frac{\gamma\left(\frac{\boldsymbol{\beta}+2\boldsymbol{\omega_0}}{2}\right)}{\mathbf{64}}\left(\left(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\right)\tilde{\rho}_A\left(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\right)\right.$$
$$\left.-\frac{1}{2}\left\{\left(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\right)\left(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\right),\tilde{\rho}_A\right\}\right)$$
$$+\frac{\gamma\left(-\frac{\boldsymbol{\beta}+2\boldsymbol{\omega_0}}{2}\right)}{\mathbf{64}}\left(\left(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\right)\tilde{\rho}_A\left(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\right)\right.$$
$$\left.-\frac{1}{2}\left\{\left(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\right)\left(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\right),\tilde{\rho}_A\right\}\right) \quad (34)$$

Having quantum master equation at hand is half of task: solution of master equation Eq. (34) (to be presented elsewhere) is needed for further use and analysis. We will now briefly comment on possible approaches in this regard.

The obtained master equation is local in time, with time-independent decay rates and Lindblad operators. Nevertheless, solving this equation is associated with some computational challenges.

By the solution of the master equation, we refer to the Kraus decomposition (RIVAS and HUELGA, 2011):

$$\rho(t)=\sum_{i=1}^{d^2}K_i(t)\rho(0)K_i^{\dagger}(t), \quad (35)$$

which follows from Kraus' theorem, which asserts that any CPTP dynamics can be cast in the above form. $K_i(t)$ are so-called Kraus' operators, while d denotes dimension of state space of open quantum system.

The method for obtaining Kraus decomposition when the master equation is known (and vice versa) is presented in (ANDERSSON *et al.*, 2007). It turns out that, in the case of three qubits considered in this paper, the method involves the use of 64×64 matrices with highly complex matrix elements, which poses a computational challenge even for specialized mathematical software. In other words, dimension of the problem increases exponentially with the system size. Obtaining Kraus decomposition is preferable whenever an assessment or verification of the algebraic properties of the dynamics of an open quantum system is required, irrespective of the physical aspects of interest — be they thermodynamic, optical, of any other nature.

Otherwise, the quantum master equation can be solved using numerical methods. Let us mention two possibilities. Using the procedure known as *quantum unravelling of the master equation* (BREUER and PETRUCCIONE, 2002) has advantage that instead working with the statistical operator everything shifts to the wave functions (each of them undergoing "quantum trajectory"). In this way, saving in computational resources is quadratic: from $\sim d^2$ parameters for density matrix to $\sim d$ parameters for wave function. This is especially convenient for finite-dimensional quantum systems: it is relatively easy to make computations using methods of numerical linear algebra.

On the other hand, quantum master equation can be expressed by systems of partial differential equations. One of the most popular approaches for solving systems of partial differential equations is the 4th-order Runge-Kutta algorithm. By integrating master equation, the density operator of open quantum system can be obtained at any time t. Some details about this and other numerical algorithms can be found in (PRESS *et al.*, 2007), with a discussion of the advantages and limitations of the methods. Of course, alternative methods and approaches found in contemporary literature also merit investigation; the discussion above is intended merely to illustrate the established procedure in the numerical solution of the master equation.

Formally, the equation Eq. (34) can also be recast in a time-dependent form, where the decay rates are specified *a priori,* based on certain phenomenological considerations, for example. This, in turn, may lead into the realm of non-Markovian dynamics through the lenses of quantum thermodynamics, to name just one possibility.

CONCLUSION

In this paper, a Markovian quantum master equation for three qubits in thermal equilibrium with the environment has been derived. The resulting master equation may be of interest for problems in e.g. quantum thermodynamics or quantum optics, within either an analytical or numerical approach.

Acknowledgments

This research is funded by the Ministry of Education and Ministry of Science, Technological Development and Innovation, Republic of Serbia, Grants no. 451-03-137/2025-03/200124 and 451-03-137/2025-03/200122.

References:

[1] ANDERSSON, E., CRESSER, J.D., HALL, M.J.W. (2007): Finding the Kraus decomposition from a master equation and vice versa. *Journal of Modern Optics* **54** (12). doi: 10.48550/arXiv.0801.4100

[2] BREUER, H.P. (2012): Foundations and Measures of Quantum Non-Markovianity. *Journal of Physics B: Atomic, Molecular and Optical Physics* **45** (15). doi: 10.48550/arXiv.1206.5346

[3] BREUER, H.P., PETRUCCIONE, F. (2002): *The Theory of Open Quantum Systems*. Oxford University Press, New York. 625 pp.

[4] CHAE, E., CHOI, J. (2024): An elementary review on basic principles and developments of qubits for quantum computing. *Nano Convergence* **11** **(**1). doi: 10.1186/s40580-024-00418-5

[5] CHRUŚCIŃSKI, D. KOSSAKOWSKI, A. (2012): Markovianity criteria for quantum evolution. *Journal of Physics B: Atomic, Molecular and Optical Physics* **45** (15). doi: 10.1088/0953-4075/45/15/154002

[6] DEJPASAND, M.T., SASANI GHAMSARI, M. (2023): Research Trends in Quantum Computers by Focusing on Qubits as Their Building Blocks. *Quantum Reports* **5** (3): 597–608. doi: 10.3390/quantum5030039

[7] GARDINER, C.W., ZOLLER P. (2004): *Quantum Noise: A Handbook of Markovian and Non-Markovian Quantum Stochastic Methods with Applications to Quantum Optics*. Springer Science & Business Media. 449 pp.

[8] JOOS, E., ZEH, H.D., KIEFER, C., GIULINI, D.J.W., KUPSCH, J., STAMATESCU, I.O. (2003): *Decoherence and the Appearance of a Classical World in Quantum Theory*. 2nd Edition. Springer-Verlag, Berlin. 496 pp. doi: 10.1007/978-3-662-05328-7

[9] MESSIAH, A. (1962): *Quantum Mechanics*. Elsevier, North Holland Publishing Company, Amsterdam. 513 pp.

[10] NIELSEN, M.A., CHUANG, I.A. (2000): *Quantum computation and quantum information*. Cambridge University Press, Cambridge. 710 pp.

[11] PRESS, W.H., TEUKOLSKY, S.A., VETTERLING, W.T., BRIAN P., FLANNERY, B.P. (2007): Numerical Recipes: The Art of Scientific Computing. 3rd. Edition. Cambridge University Press, USA. 1235 pp.

[12] RIVAS, A., HUELGA, S.F. (2011): *Open Quantum Systems – An Introduction*. SpringerBriefs in Physics. Springer Science & Business Media. 97 pp.

[13] RIVAS, A., PLATO, A.D.K., HUELGA, S.F., PLENIO, M.B. (2010): Markovian master equations: a critical study. *New Journal of Physics*, **12** (11). doi: 10.48550/ arXiv.1006.4666

[14] SCHLOSSHAUER, M. (2007): *Decoherence and the Quantum-to-Classical Transition*. Springer Science & Business Media. 416 pp. doi: 10.1007/978-3-540-35775-9

Appendix 1:

Dyadic expressions for spin-$\frac{1}{2}$ operators are given by well-known equalities:

$I = |g\rangle\langle g| + |e\rangle\langle e|$,

$S_z = \frac{\hbar}{2}(|g\rangle\langle g| - |e\rangle\langle e|)$,

$S_x = \frac{\hbar}{2}(|g\rangle\langle e| + |e\rangle\langle g|)$ and

$S_y = \frac{i\hbar}{2}(|g\rangle\langle e| - |e\rangle\langle g|)$.

From these equalities, dyadic form of spin raising and lowering operators follows:

$S_+ = S_x + iS_y = \hbar|e\rangle\langle g|$,

$S_- = S_x - iS_y = \hbar|g\rangle\langle e|$,

as well as expressions:

$|g\rangle\langle g| = \frac{1}{2}\left(I + \frac{2S_z}{\hbar}\right)$,

$|e\rangle\langle e| = \frac{1}{2}\left(I - \frac{2S_z}{\hbar}\right)$.

To meet specific requirements of calculations in this paper, it is useful to have in mind relations:

$\left(I + \frac{2S_z}{\hbar}\right)^2 = \frac{2}{\hbar}(\hbar I + 2S_z) = 4|g\rangle\langle g|$,

$\left(I - \frac{2S_z}{\hbar}\right)^2 = \frac{2}{\hbar}(\hbar I - 2S_z) = 4|e\rangle\langle e|$,

$S_-S_+ = \hbar^2|g\rangle\langle g| = \frac{\hbar^2}{2}\left(I + \frac{2S_z}{\hbar}\right)$ and

$S_+S_- = \hbar^2|e\rangle\langle e| = \frac{\hbar^2}{2}\left(I - \frac{2S_z}{\hbar}\right)$.

Appendix 2

The aim of this Appendix is to outline the derivation of expressions Eqs. (14). Having in mind that ρ_B is separable state, i.e. tensor product of density operators for each of m modes

$\rho_{B=}\rho_1 \otimes \rho_2 \ldots \otimes \rho_{\vec{k}} \ldots . \otimes \rho_{mB}$,

it follows $\langle b^{\dagger}_{\vec{k}} \rangle = tr\left[b^{\dagger}_{\vec{k}}\rho_B\right] = tr\left[b^{\dagger}_{\vec{k}}\rho_1\rho_2 \ldots \rho_{\vec{k}} \ldots . \rho_{mB}\right] = tr\left[b^{\dagger}_{\vec{k}}\rho_{\vec{k}}\right]$, where the identity $tr[A_1 \otimes A_2 \ldots \otimes A_m] = trA_1 trA_2 \ldots trA_m$ is used and the fact that $tr\left[\rho_{B\vec{k}}\right] = 1, \forall \vec{k}$.

With use of the explicit form of density operator for mode with frequency $\omega_{\vec{k}}$:

$\rho_{\vec{k}} = \sum_{k=0}^{\infty} e^{-\frac{\hbar\omega_{\vec{k}} n_{\vec{k}}}{k_B T}} |n_{\vec{k}}\rangle\langle n_{\vec{k}}|$,

the average value is:

$$\langle b^{\dagger}_{\vec{k}} \rangle = \sum_{k=0}^{\infty} \left\langle n_{\vec{k}} \left| b^{\dagger}_{\vec{k}} e^{-\frac{\hbar\omega_{\vec{k}} n_{\vec{k}}}{k_B T}} \right| n_{\vec{k}} \right\rangle = 0, \tag{A2.1}$$

by virtue of creation operator properties. In similar way it is possible to show that $\langle b_{\vec{k}} \rangle = 0$.

By definition, $\langle b^{\dagger}_{\vec{k}} b_{\vec{k}'} \rangle = tr\left[b^{\dagger}_{\vec{k}} b_{\vec{k}'} \rho_B\right]$ and using separability of state ρ_B follows:

$$\langle b^{\dagger}_{\vec{k}} b_{\vec{k}'} \rangle = tr\left[b^{\dagger}_{\vec{k}} b_{\vec{k}'} \rho_1\rho_2 \ldots \rho_{\vec{k}}\rho_{\vec{k}'} \ldots . \rho_{mB}\right] = tr\left[b^{\dagger}_{\vec{k}}\rho_{\vec{k}} b_{\vec{k}'}\rho_{\vec{k}'}\right] = \langle b^{\dagger}_{\vec{k}} \rangle \langle b_{\vec{k}'} \rangle = 0.$$

In case of $\vec{k} = \vec{k}'$:

$\langle b^{\dagger}_{\vec{k}} b_{\vec{k}} \rangle \stackrel{\text{def}}{=} \langle n_{\vec{k}} \rangle = tr\left[b^{\dagger}_{\vec{k}} b_{\vec{k}} \rho_B\right] = \frac{1}{Z}\sum_{k=0}^{\infty} n_k e^{-\frac{\hbar\omega_k n_k}{k_B T}} = \frac{1}{e^{\frac{\hbar\omega_{\vec{k}}}{k_B T}} - 1}$, so, in one place:

$$\langle b^{\dagger}_{\vec{k}} b_{\vec{k}'} \rangle = \langle n_{\vec{k}} \rangle \, \delta_{\vec{k}\vec{k}'}. \tag{A2.2}$$

Using commutator relation $\left[b_{\vec{k}}, b^{\dagger}_{\vec{k}'}\right] = \delta_{\vec{k}\vec{k}'}$ with (A2.2) follows the equality: $\langle b_{\vec{k}} b^{\dagger}_{\vec{k}'} \rangle = \left(1 + \langle n_{\vec{k}} \rangle\right) \delta_{\vec{k}\vec{k}'}$.

The rest of identities can be obtained by similar line of reasoning.