Invitation to quantum dynamical semigroups

Robert Alicki

Institute of Theoretical Physics and Astrophysics, University of Gda´nsk, Wita Stwosza 57, PL 80-952 Gda´nsk, Poland

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The theory of quantum dynamical semigroups within the mathematically rigorous framework of completely positive dynamical maps is reviewed. First, the axiomatic approach which deals with phenomenological constructions and general mathematical structures is discussed. Then basic derivation schemes of the constructive approach including singular coupling, weak coupling and low density limits are presented in their highly simplified versions. Two-level system coupled to a heat bath, damped harmonic oscillator, models of decoherence, quantum Brownian particle and Bloch-Boltzmann equations are used as illustrations of the general theory. Physical and mathematical limitations of the quantum open system theory, the validity of Markovian approximation and alternative approaches are discussed also.

I. INTRODUCTION

Classical theory of systems interacting with environment employs evolution equations which can be written in the following abstract mathematical form

$$\frac{d}{dt}p_t = \mathcal{L}p_t , \quad t \geq 0 .$$

(1)

Here \(p_t\) is a time dependent probability distribution over the relevant system’s configuration space \(\Omega\). In particular \(\Omega\) can be either a phase-space of a system, its position or momentum (velocity) space or a discrete set in the case of coarse-grained description or a discretized model. The most general “continuous” form of \(\mathcal{L}\) is a sum of a differential operator (Fokker-Planck or diffusion type) and a collisional integral one [1]. For a discrete version we can write (1) as a Pauli master equation

$$\frac{d}{dt}p_t(k) = \sum_l \left( a_{kl} p_t(l) - a_{lk} p_t(k) \right) .$$

(2)

The "gain − loss" structure of the RHS of (2) guarantees preservation of \(\sum_k p_t(k)\) while positivity of the transition probabilities per unit time \((a_{kl} \geq 0)\) implies \(p_t(k) \geq 0\). Similar mathematical consistency conditions are satisfied for the continuous cases due to the positivity of the diffusion constant (or positively defined diffusion matrix) and/or positivity of the scattering cross-sections. The solution of eq.(1) is given in terms of a Markov semigroup

$$T_t = \exp\{t\mathcal{L}\}$$

satisfying the composition law

$$T_t T_s = T_{t+s} , \quad t, s \geq 0$$

(3)

and preserving positivity and normalization of the probability distribution \(p_t\).

In the end of 60-ties and beginning of 70-ties one needed an analogical formalism to describe a variety of irreversible phenomena in quantum optics, solid state physics, magnetic resonance, nuclear and particle physics, etc. [2,3]. The classical probability distribution \(p_t\) should be replaced by the density matrix \(\rho_t\) satisfying the analog of eq.(1)

$$\frac{d}{dt}\rho_t = \mathcal{L}\rho_t , \quad t \geq 0 .$$

(4)

Besides many heuristic attempts the mathematically sound theory of quantum dynamical semigroups has been developed very soon [4-7]. It is convenient for the further discussion to distinguish two approaches in this theory - the axiomatic and the constructive one.

The former approach, presented in the next Section, is concentrated on general mathematical properties of eq.(4) and its solutions which are by no means trivial and lead to the theory of completely positive maps and semigroups on operator algebras. The fundamental structural theorems will be given and illustrated by several examples.
In constructive approach one tries to derive eq.(4) from first principles. Starting with a model of a quantum system interacting with a quantum environment one obtains Markovian master equation (4) as an approximation to the exact reduced dynamics of the open system. The canonical models of reservoirs and basic approximation procedures are discussed in Section III.

In the recent years quantum theory of open systems and in particular quantum dynamical semigroups became again a subject of intensive investigations. This is motivated by the new experimental techniques which allow precise monitoring of decoherence and dissipation in microscopic and mesoscopic quantum systems [8]. Possible future applications of controlled quantum systems in quantum information processing and quantum computing are another sources of this revival [9]. Both mentioned above approaches are necessary to create physically correct, mathematically consistent and convenient for practical applications theory.

The number of publications on this topic is enormous and therefore the presented list of references is far from being complete, often review papers, books and other contributions to this volume are quoted instead of the original papers.

II. AXIOMATIC APPROACH

Consider an open quantum system with the associated Hilbert space \( \mathcal{H} \) with the time evolution governed by the master equation (4) for its density matrix \( \rho_t \). This is the Schrödinger picture of a time evolution which will be used in this paper. We leave as a simple exercise for the reader to translate all the presented results to the Heisenberg picture.

In order to give a precise mathematical meaning to eq.(4) we first extent it to the whole Banach space \( T(\mathcal{H}) \) of trace-class operators acting on \( \mathcal{H} \) equipped with the norm \( ||\sigma||_1 = \text{tr}(\sigma\sigma^*)^{1/2} \). Then \( L \) is a linear, perhaps unbounded, operator defined on its domain \( D(L) \subset T(\mathcal{H}) \). The formal solution of eq.(4) is given by the the one-parameter semigroup \( \Lambda_t, t \geq 0 \)

\[
\Lambda_t \sigma = \sum_{n=0}^{\infty} \frac{t^n}{n!} L^n \sigma
\]

for a bounded operator \( L \) while for an unbounded one

\[
\Lambda_t \sigma = \lim_{n \to \infty} (1 - tL)^{-n} \sigma
\]

makes sense. The semigroup \( \Lambda_t \) should satisfy the following conditions

\[
\Lambda_t \Lambda_s = \Lambda_{t+s} \quad \text{semigroup property}
\]

\[
\lim_{t \to +0} \Lambda_t \sigma = \sigma \quad \text{continuity}
\]

for \( \sigma \geq 0 \), \( \Lambda_t \sigma \geq 0 \) \quad \text{positivity}

\[
\text{for any } \sigma \in T(\mathcal{H}) , \text{ Tr } (\Lambda_t \sigma) = \text{Tr } \sigma \quad \text{trace preservation} .
\]

We shall see that the particular feature of composed quantum systems, namely the existence of entangled states, makes us to replace the positivity condition (9) by a stronger one called complete positivity.

A. Complete positivity

Consider two well-separated open quantum systems with dynamics given by two dynamical maps \( \Lambda^{(1)} \) and \( \Lambda^{(2)} \) respectively. Assume also that the initial state of a joined system is determined by the entangled density matrix

\[
\rho^{(12)} \neq \sum_j p_j \rho^{(1)}_j \otimes \rho^{(2)}_j .
\]

One can easily find examples (e.g. for 2 qubits) of positive trace preserving \( \Lambda^{(1)} \) and \( \Lambda^{(2)} \) and \( \rho^{(12)} \) satisfying (11) such that \( \Lambda^{(1)} \otimes \Lambda^{(2)} \rho^{(12)} \) is not positively defined [10]. The minimal condition which must be imposed on dynamical
maps to allow meaningful tensor products is complete positivity which means that for any \( n = 1, 2, 3, \ldots \), \( \Lambda \otimes I_n \) is positive, where \( I_n \) is an identity map acting on \( n \times n \) matrices (i.e. trivial dynamical map on \( n \)-level quantum system). Completely positive maps on operator algebras were studied already in the 50-ties and the celebrated Stinespring representation [11] leads to a general form of completely positive dynamical map called often Kraus decomposition [12]

\[
\Lambda \rho = \sum_{\alpha} W_{\alpha} \rho W_{\alpha}^* 
\]

where \( W_{\alpha} \) are bounded operators on \( \mathcal{H} \) satisfying \( \sum_{\alpha} W_{\alpha}^* W_{\alpha} = 1 \). The decomposition (12) is highly nonunique, in particular the sum over \( \alpha \) can be replaced by an integral. If \( \mathcal{H} \) is \( n \)-dimensional then one can always find Kraus decomposition in terms of at most \( n^2 \) terms.

\section*{B. Completely positive dynamical semigroups}

From now on by a quantum dynamical semigroup (QDS) we mean a family of maps \( \Lambda_t, t \geq 0 \) satisfying conditions (7)-(10) with (9) strengthened to complete positivity. The celebrated result of Lindblad, Gorini, Kossakowski and Sudarshan [4,5] provides us with the most general form of a quantum Markovian master equation (MME) with a bounded generator

\[
\frac{d}{dt} \rho_t = -i[H, \rho_t] + \sum_j V_j \rho_t V_j^* - \frac{1}{2} \{ \sum_j V_j^* V_j, \rho_t \} .
\]

or in a slightly different but often used form

\[
\frac{d}{dt} \rho_t = -i[H, \rho_t] + \frac{1}{2} \sum_j \{ |V_j, \rho_t V_j^*| + |V_j^* \rho_t, V_j| \} .
\]

The choice of bounded operators \( H = H^* \) and \( V_j \) is again not unique and the sum over \( \{j\} \) can be replaced by an integral. To simplify the notation we put always \( \hbar = 1 \) and \( k_B \equiv 1 \) to have the same units for energy, frequency and temperature.

The non-Hamiltonian part of the generator (13) displays the "gain - loss" structure similar to that of Pauli master equation (2) and determined by a completely positive quantum transition map

\[
\rho \mapsto \Phi \rho = \sum_j V_j \rho V_j^*
\]

which is a sum of "pure" transition maps \( \rho \mapsto V_j \rho V_j^* \) corresponding to elementary irreversible processes [7].

The following expansion for \( \Lambda_t = \exp(tL) \) involving only sums (or integrals) and compositions of manifestly completely positive maps \( \Phi \) (15) and \( W_t \)

\[
W_t \rho = S_t \rho S_t^* , \quad S_t = \exp\{ -itH - (t/2) \sum_j V_j^* V_j \}
\]

is often useful

\[
\Lambda_t = W_t + \sum_{n=1}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \ldots \int_0^{t_2} dt_1 W_{t-t_n} \Phi W_{t_{n-1}-t_n} \Phi \ldots W_{t_2-t_1} \Phi W_{t_1} .
\]

For open systems with infinite dimensional Hilbert spaces we expect that the generators of QDS are typically unbounded. Although there exists no theorem giving the most general structure of \( L \) in this case, the standard form (13)(14) makes sense very often [13,14]. Then the operators \( H \) and \( V_j \) can be unbounded, in fact \( V_j \) can be even operator-valued distributions (e.g. quantum fields) and the sum over \( \{j\} \) can be replaced by an integral. The typical mathematical condition which could be imposed is the existence of the contacting semigroup \( S_t \) (16) on the Hilbert space such that the operators \( S_t V_j \) became bounded and the expansion (17) makes sense. One of the unexpected features of the solutions to MME with unbounded generators is that despite the formal trace preservation of (13)(14) we can have \( \text{Tr} \rho_t < \text{Tr} \rho_0 \). This phenomenon is known for classical Pauli master equations with infinite number of states where for certain transition probabilities "the system can escape to infinity in finite time" [15].
C. Examples

We present few examples of QDS generators obtained using axiomatic construction based on phenomenological arguments. For other interesting models of dissipative quantum systems studied using numerical computations also, see [16].

1. 2-level system

The simplest and the oldest example of QDS for a 2-level system (qubit) can be constructed using three elementary transition maps. Assume that $|1\rangle$ and $|2\rangle$ form a basis of Hamiltonian eigenvectors and define the following operators

$$P_k = |k\rangle\langle k|, \ k = 1, 2, \ \sigma^+ = (\sigma^-)^* = |2\rangle\langle 1|, \ \sigma_3 = P_2 - P_1.$$ (18)

The transition maps correspond to three different irreversible processes

- damping $\rho \mapsto \gamma_1 \sigma^- \rho \sigma^+$
- pumping $\rho \mapsto \gamma_1 \sigma^+ \rho \sigma^-$
- pure decoherence $\rho \mapsto \delta_1 P_1 \rho P_1 + P_2 \rho P_2$. (21)

The master equation obtained from (18)-(21) reads

$$\frac{d}{dt}\rho_t = -\frac{i\omega}{2}[\sigma_3, \rho_t] + \frac{\gamma_1}{2}([\sigma^-, \rho_t \sigma^+] + [\sigma^- \rho_t, \sigma^+]) + \frac{\gamma_1}{2}([\sigma^+, \rho_t \sigma^-] + [\sigma^+ \rho_t, \sigma^-]) - \frac{\delta}{2}[[\sigma_3, \sigma_3], \rho_t]$$ (22)

where $\delta = (\delta_1 + \delta_2)/2$. Using the decomposition

$$\rho_t = p_1(t)P_1 + (1 - p_1(t))P_2 + \alpha(t)\sigma^+ + \bar{\alpha}(t)\sigma^-$$ (23)

we obtain

$$p_1(t) = p_1(0)e^{-(\gamma_1 + \gamma_1)t} + \frac{\gamma_1}{\gamma_1 + \gamma_1}(1 - e^{-(\gamma_1 + \gamma_1)t})$$

$$\alpha(t) = \alpha(0)\exp\{-i\omega t - (\gamma_1 + \gamma_1 + \delta)t/2\}.$$ (24)

The diagonal elements of $\rho_t$ evolve independently of the off-diagonal ones and the former satisfy Pauli master equation with a stationary state which can be written in a form of the Gibbs state

$$\rho_{eq} = (2 \cosh \frac{\omega}{2T})^{-1} e^{-\omega \sigma_3 / 2T}, \ \frac{\gamma_1}{\gamma_1} = e^{-\omega / T}.$$ (25)

Moreover, for any initial state $\rho_t \rightarrow \rho_{eq}$ for $t \rightarrow \infty$ and the generator satisfies quantum detailed balance condition.

The equation (22) written explicitly in terms of matrix elements is called Bloch equation and is frequently used in quantum optics and magnetic resonance theory.

2. Harmonic oscillator

Another well-known example is a linearly damped and pumped harmonic oscillator with a Hamiltonian $H = \omega a^+ a$ ($[a, a^+] = 1$) and transition maps describing coherent damping and pumping

- damping $\rho \mapsto \gamma_1 a \rho a^+$
- pumping $\rho \mapsto \gamma_1 a^+ \rho a$. (26)

The master equation with an unbounded generator

$$\frac{d}{dt}\rho_t = -i\omega[a^+ a, \rho_t] + \frac{\gamma_1}{2}([a, \rho_t a^+] + [a \rho_t, a^+]) + \frac{\gamma_1}{2}([a^+, \rho_t a] + [a^+ \rho_t, a])$$ (27)
is exactly solvable and the solution can be presented for instance in the form of the quantum generating function of the complex variables \( z, \bar{z} \) [7]

\[
F_t(z, \bar{z}) = \text{Tr}(\rho_t \exp\{za - \bar{z}a^+\}) = e^{-A(t)} F_0(z_t, \bar{z}_t)
\] (28)

where

\[
z_t = z \exp\{-i\omega t - (\gamma_\downarrow - \gamma_\uparrow) t/2\}, \quad A(t) = \frac{|z|^2}{4} \frac{\gamma_\uparrow}{\gamma_\downarrow - \gamma_\uparrow} \left(1 - e^{-(\gamma_\downarrow - \gamma_\uparrow)t}\right).
\] (29)

By differentiation of \( F_t(z, \bar{z}) \) with respect to \( z \) or \( \bar{z} \) one obtains time dependence of all moments \( \text{Tr}(\rho_t (a^+)^n a^m) \). One can see from (28)(29) that if \( \gamma_\downarrow > \gamma_\uparrow \) then \( \lim_{t \to \infty} \rho_t = \rho_{eq} \) where

\[
\rho_{eq} = (1 - e^{-\omega/T}) \exp\left\{-\frac{1}{T} \omega a^+ a\right\}, \quad \frac{\omega}{T} = \log \frac{\gamma_\downarrow}{\gamma_\uparrow}.
\] (30)

One can also show that the diagonal and off-diagonal matrix elements of \( \rho_t \) evolve independently with the former satisfying detailed balance Pauli master equation.

Equation (27) found numerous applications, for instance in quantum optics to describe single mode of radiation in cavity. This is also the simplest example of the important class of the quasi-free QDS (see [7,10] and references therein).

3. Decoherence of mass center

Following [17] we briefly present a model based on QDS which can be used to analyse environmental decoherence which cause the transition from quantum to classical world. Consider a mass center of a body described by the Hamiltonian

\[
H = \frac{1}{2M} P^2 + V(X)
\] (31)

where \( X \) and \( P \) are the operators of mass center and total momentum satisfying

\[
[X_k, P_l] = i\delta_{kl}, \quad k, l = 1, 2, 3.
\] (32)

We assume that the interaction with an environment can be reduced to processes of scattering, absorption or emission. A collision with a gas particle and emission, absorption or scattering of a photon (or other quasiparticle) causes a momentum transfer \( k \) which changes the total momentum. The following transformation (in the Heisenberg picture)

\[
e^{ikX}P e^{-ikX} = P + k
\] (33)

describes this momentum transfer independently of the detailed microscopic mechanism of energy redistribution. Therefore the elementary irreversible process is given by the transition map

\[
\rho \mapsto e^{-ikX} \rho e^{ikX}.
\] (34)

Assuming statistical independence of different momentum transfer events (called simply collisions) we obtain the following form of the MME

\[
\frac{d}{dt} \rho_t = -i[H, \rho_t] + \int_{\mathbb{R}^3} d^3k n(k) \left(e^{-ikX} \rho_t e^{ikX} - \rho_t\right)
\] (35)

where \( n(k) \) is a density of collisions per unit time leading to the momentum transfer \( k \).

The generator given by (35) takes into account momentum conservation but the average kinetic energy grows to infinity for \( t \to \infty \) and hence the process of ultimate relaxation to equilibrium is not properly described. However, it is expected that in the limit of large mass \( M \) and for slowly varying potential \( V(X) \) the decoherence time is much shorter than the energy dissipation time scale. Therefore the master equation (35) can be considered as a good approximation for the study of pure decoherence in the relevant regime of large body at slowly varying potential and rare collisions (see Section III. D.3).
4. Bloch-Boltzmann equation

In quantum optics the investigation of an active atom interacting with radiation and immersed in the thermal bath of perturbers (typically, noble gas atoms) is a very important topic [18]. To simplify the description one assumes that the spatially uniform distribution of active atoms and strong decoherence due to collisions with perturbers justify the use of the density operators diagonal in momentum (or velocity) representation. Therefore, we consider a family $\rho(t) \geq 0$ of velocity-dependent positively defined operators (matrices) acting on the Hilbert space describing the internal structure of an active $n$-level atom. Using a standard form of the master equation (13) one can easily derive the most general evolution equation for QDS which preserves such partially diagonal structure of the density matrix [19]. It reads

$$\frac{d}{dt} \rho_t(v) = -i \sum_a \hbar(a(v)[S_a, \rho_t(v)] + \sum_{a,b} \int_{\mathbb{R}^3} d^3v' \mathcal{K}_{ab}(v; v') S_a \rho_t(v') S_b^* - \frac{1}{2} \sum_{a,b} \gamma_{ab}(v) \{S_a^* S_b, \rho_t(v)\}$$

(36)

where $\{S_a\}$ form a linear basis in the space of $n \times n$ matrices and

$$\text{for any } v, v', \quad \mathcal{K}_{ab}(v; v') \text{ is positively defined}, \quad \gamma_{ab}(v) = \int_{\mathbb{R}^3} d^3v' \mathcal{K}_{ba}(v; v') .$$

(37)

Equation (36) provides an example of a classical-quantum description which combines a generalisation to $n$-level case of the MME (22), called Bloch equation with a classical linear Boltzmann equation for spatially uniform case. Similar type of equations found applications in the quantum measurement theory [20].

D. Ito-Schrödinger equations

In the classical theory the Fokker-Planck equation describing Brownian motion in terms of probability distribution over the phase-space of Brownian particle is completely equivalent to the Langevin equation (in Ornstein-Uhlenbeck formulation) for the particle’s random trajectory. The later equation is a prototype of stochastic differential equation which can be written either in Ito or Stratonovich form [1]. The similar equivalent description exists for quantum dynamical semigroups with the generator (13) in terms of the following Ito-Schrödinger equation

$$d\psi(t) = -iH\psi(t)dt - \frac{1}{2} \sum_j V_j^* V_j \psi(t)dt - i \sum_j V_j \psi(t) dB_j(t) .$$

(38)

In (38) $B_j(t)$ denote independent and normalized Brownian motion processes and heuristically $“ dW “$ corresponds to “white noise”. The short-hand notation $df(t) = a(t)dt + b(t)dB(t)$ has a meaning of the corresponding integral equation

$$f(t_1) - f(t_2) = \int_{t_1}^{t_2} a(t)dt + \int_{t_1}^{t_2} b(t)dB(t)$$

(39)

where the second integral is an “nonanticipating” Ito integral given by the probabilistic limit of the sums $\sum b(s_k)[B(s_{k+1}) - B(s_k)]$ with $t_1 = s_1 < s_2 < \ldots < s_n = t_2$. To perform computations using stochastic integrals one applies Ito rule

$$dB_i(t)dB_j(t) = \delta_{ij} dt$$

(40)

and $E[dB_j(t)] = 0$ where $E[\cdot]$ denotes the average with respect to Brownian motions. One should remember that $dB_j(t) = B_j(t + dt) - B_j(t)$ is always statistically independent on the solution of stochastic differential equation up to time $t$. Applying those rules to the density matrix of the open system defined as an average $\rho(t) = E[|\psi(t)\rangle < \psi(t)]$ we obtain

$$d\rho_t = dE[|\psi(t)\rangle < \psi(t)] = E[d|\psi(t)\rangle < \psi(t)] + |\psi(t)\rangle < d\psi(t)| + |d\psi(t)| [< d\psi(t)]$$

$$= -i[H, \rho_t]dt - \frac{1}{2} \left\{ \sum_j V_j^* V_j, \rho_t \right\} dt + \sum_j V_j \rho_t V_j^* dt$$

(41)
that coincides with MME (13). The Ito-Schrödinger equation (38) for a general case was firstly proposed in [21,22] and then derived by different authors as a useful tool for numerical simulations of quantum open systems [23]. For such applications it is convenient to use an equivalent nonlinear modification of (38) with the normalized solutions \( \phi(t) = \psi(t)/\|\psi(t)\| \). One should notice that to obtain (41) we can replace the Brownian motions \( B_j(t) \) by arbitrary stochastic processes \( X_j(t) \) (continuous or jump processes) with independent increments such that \( E[dX_i(t)dX_j(t)] = \delta_{ij}dt \). The different processes represent unitarily equivalent representations of the singular reservoirs constructed in terms of “time ordered Fock spaces” [21]. Possible physical interpretations of these different representations are discussed in [24].

An alternative approach in terms of “quantum noises” has been proposed in [25] and subsequently developed into a mathematically rigorous theory of noncommutative stochastic differential equations.

E. Problems and pitfalls

Although, the axiomatic approach allows to write down the MME (13,14) in a mathematically consistent form, we generally need additional phenomenological insights which could lead to concrete form of the operators \{\( V_j \}\}. The first problem is the relation between the dissipative part in (13,14) and the Hamiltonian of the open system. Here the demanded structure of the stationary state and detailed balance condition are helpful [7]. For example adding a nonlinear term to the Hamiltonian of the harmonic oscillator we have to modify the dissipative part too, in contrast to often used simplified models with linear dissipation. The symmetries of the system and reservoir give another restrictions on the form of generators [26].

For many interesting physical problems we have to include time dependent-external fields acting on the system. Very often it is done by simply adding the proper time-dependent term to the Hamiltonian without changing the dissipative part. This can be justified, however, for weak and quickly oscillating fields while in general case the whole Markovian approximation breaks down [27]. Another extreme case is a slowly varying external potential which leads to a proper time-dependent generator which for any time reproduces, for example, return to an equilibrium state given by a total instant Hamiltonian [28].

A particular care is needed when we put two open systems \( S_1, S_2 \) with their “privat” reservoirs \( R_1, R_2 \) into contact by adding their interaction Hamiltonian \( V_{12} \). In this case we cannot simply add two dissipative generators obtained previously for decoupled systems \( S_1, S_2 \). This is obvious for the case of two heat baths at the same temperature which should drive the interacting system \( S_1 + S_2 \) into its Gibbs state which of course depends on the new element \( V_{12} \).

III. CONSTRUCTIVE APPROACH

The goal of the constructive approach is to derive, using mathematically controlled approximations, Markovian dynamics of the quantum system interacting with the quantum environment. We restrict ourselves to the derivations which respect complete positivity of the reduced dynamics. In author’s opinion the very scheme of quantum open systems approach and particularly Markovian approximations are consistent only under well defined conditions discussed below.

A. Basic assumptions

In the theory of quantum open systems we decompose the Universe into three parts \( (S,O,R) \). The first one is an open system \( S \) controlled by an ”active” observer \( O \) and interacting with the ”passive” rest \( R \) which is called reservoir. If the state of the system \( S + R \) is given by the density matrix \( \rho_{SR} \) that we assume that the reduced density matrix \( \rho_S = \text{Tr}_R \rho_{SR} \) possesses an operational meaning i.e. that the observer \( O \) can prepare an arbitrary initial state of \( S \) at a certain moment \( t_0 = 0 \) and than measure the evolved state at the moment \( t > 0 \). We often assume also that the observer can control to some extend the evolution of \( S \) switching-on external time-dependent ”fields”. The physical structure of \( O \) and the description of measurements performed na \( S \) is a subject of quantum measurement theory and will be not discussed here.

One should notice that the above scheme contains a tacit assumption that the interaction between \( S \) and \( R \) is weak. Any preparation of the initial state of \( S \) or its state measurement takes time \( t_p = \hbar/\delta E \) where \( \delta E \) is an energy resolution of state preparation or measurement. For a quantum system \( S \) with a discrete spectrum \( \delta E \) should
be smaller that the typical separation between the energy levels while for systems with continuous spectrum (e.g. quantum Brownian particle) \( t_p \) is directly related to a chosen time-scale of observation (see Section III.D.3). Obviously, during preparation or measurement processes the system \( S \) should not be strongly perturbed by the environment \( R \) what implies the inequality

\[
t_p << \tau_S
\]

where \( \tau_S \) is a characteristic time scale of relaxation of \( S \) due to the interaction with \( R \).

The first step towards mathematical description of the open system consists in writing down the formal "bare" Hamiltonian

\[
H_{SR} = H^0_S + \lambda \sum_k S_k \otimes R^0_k + H_R
\]

where \( H^0_S \) is a bare Hamiltonian of \( S \), the interaction term is proportional to a dimensionless coupling constant \( \lambda \) and contains bare reservoir’s operators \( R^0_k \). For some applications we shall add a time-dependent contribution \( V(t) \) to the Hamiltonian \( H^0_S \) in order to take into account external fields used by the observer \( O \) to control our system \( S \).

The next important assumption is the product structure of the initial state for \( S + R \)

\[
\rho_{SR}(0) = \rho \otimes \omega_R
\]

with an arbitrarily prepared initial state of \( S \) and a fixed reference state of \( R \). Again this assumption can be justified if the interaction is weak in a defined below sense [29]. Namely, the system \( S + R \) for times preceding the preparation at \( t_0 = 0 \) is expected to be at equilibrium or ground state \( \omega_{SR} \). In order to produce the initial state (44) by applying external perturbations to \( S \) we must assume that

\[
\omega_{SR} \simeq \omega_S \otimes \omega_R.
\]

The state of \( S \) for times \( t >> t_p \) is then given by the reduced density matrix (we omit subscript \( S \))

\[
\rho_t = \text{Tr}_R(U_t \rho \otimes \omega_R U^*_t) = \Lambda_t(\rho)
\]

where \( U_t = \exp(-iH_{SR}) \) and \( \text{Tr}_R \) is a partial trace over the Hilbert space of \( R \). The dynamical maps \( \{ \Lambda_t; t \geq 0 \} \) are by construction completely positive and trace preserving.

However, the practical implementation of the above prescription leads to difficulties. Take as an example, a model of atom interacting with electromagnetic field at zero temperature. The corresponding Hamiltonian (43) is well-defined only if an ultraviolet cut-off at the frequency \( \omega_c \) is introduced replacing "bare" operators \( R^0_k \) by cut-off dependent regularized \( R_k \). Then a simple lowest order evaluation of (46) shows that the interaction produces a cut-off dependend Hamiltonian correction to the bare Hamiltonian \( H^0_S \). When \( \omega_c \to \infty \) corrections diverge and must be cancelled by proper counterterms in the bare Hamiltonian (renormalization procedure). In the case of our example it leads to mass and charge renormalization and slight modification of the Coulomb potential which influences energy levels of the atom (Lamb-shift)[30]. A different example is an electron immersed into a polar solid. The interaction with lattice ions modelled by the electron-phonon coupling (with natural well-defined cut-off) completely changes the properties of an electron leading to the so-called polaron model. In both cases the initial bare system is strongly modified by a "cloud" which consists of certain degrees of freedom of the reservoir [31]. Hence the decomposition into \( S + R \) is not unique and the practical criterion should be the weakness of the residual interaction between the "dressed" system \( S' \) and the rest of the reservoir \( R' \). Practically, we describe the sytems \( S', R' \) by the same Hilbert spaces as \( S, R \) and the Hamiltonian of the bath \( H_R \) remains the same too. We introduce, however, a physical (renormalized) Hamiltonian \( H_S \) and modify the structure of interaction Hamiltonian introducing suitable formfactors with cut-offs and often leaving only resonant terms ("rotating wave approximation" in quantum optics, Lee models in particle physics) to reduce creation of the "cloud". We shall illustrate these problems later on in the case of 2-level open system (see Sections III.C.2, III.D.2).

B. Models of reservoirs

Similarly to the classical case represented by the standard example of Brownian motion the details of the reservoir should not be essential for the dynamical behaviour of an open system \( S \) at least on the proper "coarse-grained"
which is relevant for different Markovian regimes. Introducing the reservoir’s relaxation time scale $V$ stochastic Ito-Schrödinger equation (38) with to include the averaging effect of the Hamiltonian dynamics of $S$ in order to satisfy (51). Moreover, rigorous analysis shows that the Markovian approximation needs also sufficiently rapid decay of higher order multitime correlation functions which can be proved for quasi-free models of reservoirs discussed in the previous subsection.

C. Markovian limits

The general reduced dynamics (46) does not satisfy the semigroup composition law (7). However, one expects that at least for a certain coarse-grained time scale, roughly determined by $\tau_S$ (see (42)), this law is often a very good approximation. Physically, it is true if the exact state of the system $S + R$ given by $U_t \rho \otimes \omega_R U_t^*$ does not differ locally from the state $\Lambda_t(\rho) \otimes \omega_R$. Here ”locality” is determined by the radius of interaction between $S$ and $R$. Mathematically this condition can be expressed as a sufficiently fast decay of the reservoirs correlation functions

$$R_{kl}(t) = \text{Tr}(\omega_R R_k(s + t) R_l(s))$$

where $R_k(t) = \exp(itH_R)R_k\exp(-itH_R)$ and we assume that the reservoir’s reference state $\omega_R$ is stationary with respect to its evolution. We shall argue that those correlation functions contain the total information about reservoirs which is relevant for different Markovian regimes. Introducing the reservoir’s relaxation time scale $\tau_R$ we may write the standard condition for the validity of the Markovian approximation as

$$\tau_R << \tau_S .$$

However, as we shall see, important examples of reservoirs may not have a natural decay time scale $\tau_R$ and one has to include the averaging effect of the Hamiltonian dynamics of $S$ in order to satisfy (51). Moreover, rigorous analysis shows that the Markovian approximation needs also sufficiently rapid decay of higher order multitime correlation functions which can be proved for quasi-free models of reservoirs discussed in the previous subsection.
In the present review we are not going to reproduce involved rigorous derivations which can be found in the literature [34-36]. Our aim is to discuss physical assumptions behind different Markovian regimes and proper approximation schemes based on the relevant order of perturbation which yield mathematically consistent results. For notational simplicity we use as an illustration the model of an effective 2-level open system with a physical (renormalized) Hamiltonian $H_S$ and the interaction one $H_{\text{int}}$ of the form

$$H_S = \frac{1}{2} \epsilon \sigma_3 , \quad H_{\text{int}} = \lambda \sigma_1 \otimes R \quad (52)$$

where $\sigma_k, k = 1, 2, 3$ are Pauli matrices. We always assume that

$$\text{Tr}(\omega R) = 0 . \quad (53)$$

In the heuristic derivations of MME the lowest order expansion for quantum dynamical semigroup of the form

$$\rho_t = e^{-itH_S}(\rho + \sum_j \int_0^t V_j(s) \rho V_j^*(s) - \frac{1}{2} \{V_j^*(s)V_j(s), \rho\} ds)e^{itH_S} + O(t^2) \quad (54)$$

is compared with the relevant term in the expansion for the reduced dynamics (46). More precisely, it is enough to compare only the transition map term ("gain")

$$\rho \mapsto \sum_j \int_0^t V_j(s) \rho V_j^*(s) ds \quad (55)$$

with the corresponding expression obtained from (46) using different assumption concerning mainly important time scales in the joint system $S + R$. Any Hamiltonian-type corrections are put equal to zero according to the renormalization procedure.

1. **Singular coupling or white noise Anzatz**

Using second order Dyson expansion for the total dynamics of $S + R$ with the interaction Hamiltonian treated as a perturbation we obtain the following formula for the manifestly completely positive "transition map" which has to be compared with (55)

$$\rho \mapsto \int_0^t ds_1 \int_0^t ds_2 \text{Tr}(H_{\text{int}}(s_1) \rho \otimes \omega R H_{\text{int}}(s_2)) \quad (56)$$

For our 2-level system we obtain

$$\rho \mapsto \lambda^2 \int_0^t ds_1 \int_0^t ds_2 R(s_2 - s_1) \left(e^{i\epsilon(s_2-s_1)} \sigma_3 \rho \sigma_3^+ + e^{-i\epsilon(s_2-s_1)} \sigma_3 \rho + e^{i\epsilon(s_2+s_1)} \sigma_3 \rho \sigma_3^+ + e^{-i\epsilon(s_2+s_1)} \sigma_3 \rho \sigma_3^+ \right) \quad (57)$$

The simplest approximation which produces the Markovian transition map term (55) is based on the assumption that the correlation time of the reservoir is much shorter than any other relevant time scale i.e.

$$\tau_R << \min\{\tau_S, \tau_H\} \quad (58)$$

where $\tau_H$ denotes Heisenberg time scale for $S$ related to the average energy level spacing $\Delta E$ by $\tau_H = (\Delta E)^{-1}$. Under the condition (58) we can use the white-noise Anzatz

$$R(t) \simeq \hat{R}(0) \delta(t) , \quad \hat{R}(\omega) = \int_{-\infty}^{\infty} R(t)e^{i\omega t} dt \quad (59)$$

which leads to the QDS-type of the transition map corresponding to the following MME

$$\frac{d}{dt} \rho = -\frac{i}{2} [\sigma_3, \rho] - \frac{\lambda^2}{2} \hat{R}(0) [\sigma_1, [\sigma_1, \rho]] . \quad (60)$$
For a general case the substitution of the type (59) leads to MME (13,14) with \( V_j = V_j^* \) which can be rewritten in a \textit{double commutator form}. Moreover, the dissipative part does not depend on the Hamiltonian one and we can even add a time-dependent term \( V(t) \) to obtain

\[
\frac{d}{dt} \rho_t = -i[(H_S + V(t)), \rho_t] - \frac{1}{2} \sum_j [V_j, [V_j, \rho_t]] .
\] (61)

The dynamics generated by (61) is very special because the dynamical maps \( \Lambda_t \) are \textit{bistochastic}, i.e. \( \Lambda_t \mathbf{1} = \mathbf{1} \). It means, depending on the physical context, that the \textit{infinite temperature} or \textit{microcanonical} state is preserved and the H-theorem holds i.e. for any solution of (61)\[37\]

\[
S(\rho_t) \geq S(\rho_s) , \text{for } t \geq s \geq 0 , \quad S(\rho) = -\text{Tr} \ln \rho .
\] (62)

There are several instances where the equations of type (61) are useful and provide reasonable approximations to the exact dynamics of the open system. These are the cases where the Hamiltonian self-evolution due to \( H_S + V(t) \) is very slow or \( H_S + V(t) \) commutes with \( S_k \) in (43) and therefore the pure decoherence processes dominate over the energy redistribution. Another case is the high temperature limit where \( T > E_{\text{max}} \) and \( E_{\text{max}} \) is a maximal difference of energy levels of the system. The white noise Anzatz can be obtain from the Hamiltonian models by limit procedure called \textit{bistochastic coupling limit} which leads to unphysical limiting reservoirs with unbounded from below Hamiltonians [35].

One should remember, however, that the lack of memory expressed by the \( \delta \)-like correlations in (59) contradicts the quantum nature of the reservoir (see Section III.D.1) and the noise governing the dissipative part of (61) is essentially classical. Hence, in author’s opinion, equations of the type (61) are too rough to describe properly the control of decoherence and dissipation in the context of quantum computations and error correction schemes. The same is true for their discrete-time versions which often appear in the literature on this topic [9].

2. \textit{Weak coupling limit}

Another approximation scheme takes into account the interplay between the Hamiltonian dynamics of \( S \) governed by \( H_S \) and the coupling to \( R \). It allows to describe, for instance, the equilibration process leading in the case of a heat bath to a final Gibbs state of \( S \). We assume the following relations between the relevant time scales

\[
\tau_H << \tau_S , \quad \tau_R << \tau_S .
\] (63)

As a consequence of (63) in the example (57) the last two non-resonant terms can be omitted and the obtained transition map corresponds to the following MME

\[
\frac{d}{dt} \rho_t = -i[\sigma_3, \rho_t] - \frac{\lambda^2}{2} \left( \hat{R}(e)[\sigma^- \rho_t \sigma^+] + [\sigma^- \rho_t, \sigma^+] + \hat{R}(-e)[\sigma^+ \rho_t \sigma^-] + [\sigma^+ \rho_t, \sigma^-] \right) .
\] (64)

which is a special case of (22) with \( \delta = 0 \). The similar procedure applied to a harmonic oscillator linearly coupled to an environment yields MME (27)

For a general case (43) the MME obtained under the conditions (63) reads

\[
\frac{d}{dt} \rho_t = -i[H_S, \rho_t] + \frac{\lambda^2}{2} \sum_{\omega, k, l} \hat{R}_{kl}(\omega) \left( [S_k(\omega), \rho_t S_l^*(\omega)] + [S_k(\omega) \rho_t, S_l^*(\omega)] \right)
\] (65)

where

\[
S_k(t) = e^{itH_S} S_k e^{-itH_S} = \sum_{\omega} S_k(\omega) e^{-i\omega t}
\] (66)

and

\[
\hat{R}_{kl}(\omega) = \int_{-\infty}^{\infty} R_{kl}(t) e^{-i\omega t} dt .
\] (67)

Obviously, as for any eigenfrequency \( \omega \) the matrix \( [\hat{R}_{kl}(\omega)] \) is positively defined we can always rewrite (65) in a diagonal form (13,14).
The approximation procedure leading to MME (65) (in the interaction picture) can be made mathematically rigorous introducing the concept of weak coupling or van Hove limit applied to the reduced dynamics in the interaction picture which consists of using the rescaled time $\tau = \lambda^2 t$ for $\lambda \to 0$. The details can be found in [34] see also the related idea of stochastic limit in [33].

MME of the type (65) possess several interesting properties. The dissipative part of the generator commutes with the Hamiltonian one and the diagonal elements of $\rho_t$ in the energy representation evolve independently of the off-diagonal ones. The corresponding transition probabilities which appear in the Pauli master equation for diagonal elements are exactly equal to those calculated using the Fermi Golden Rule [38]. In the frequently used case of the reservoir being at thermal equilibrium (heat bath) the KMS relation of the form

$$\hat{R}_{kl}(-\omega) = e^{-\beta\omega}\hat{R}_{kl}(\omega) , \beta = T^{-1}$$

(68)

is valid and implies that that the Gibbs state $\rho_{eq} = Z^{-1} \exp\{-\beta H_S\}$ is an invariant state for MME (65). If for all $k, \omega$, $[S_k(\omega), X] = 0$ implies $X = c1$ the Gibbs state is ergodic i.e. for $t \to \infty$ and any initial state the solution of (65) $\rho_t \to \rho_{eq}$. Moreover, the Pauli master equation for the diagonal elements of $\rho_t$ satisfies detailed balance condition. The part of the generator in (65) which is given by terms with $\omega = 0$ does not influence the diagonal elements of $\rho_t$ and describes pure decoherence which is not accompanied by the energy change.

One should notice the important differences between the regimes characterized by inequalities (58) and (63) respectively. The former allows white-noise Ansatz and hence the strictly Markovian approximation entirely due to the memoryless reservoir. In the later case Markovian approximation is valid for the time evolution averaged over many periods of Hamiltonian evolution of the open system. It follows that the dissipative part of the semigroup generator strongly depends of the Hamiltonian $H_S$ and therefore we cannot freely add a time dependent part $V(t)$ to $H_S$.

3. Weak coupling and thermodynamics

We have already seen that the MME (65) obtained using weak coupling limit satisfies the 0-law of thermodynamics, namely the heat bath drives an open system $S$ to its equilibrium state at the same temperature. Introducing a time dependent Hamiltonian $H_S(t)$ which varies on the time-scale much longer than all other time-scales in (63) we can apply the same method used to derive MME (65). As a result of such combined weak-coupling and adiabatic approximation we obtain an inhomogeneous in time MME of the form

$$\frac{d}{dt}\rho_t = -i[H_S(t),\rho_t] + L_D(t)\rho_t \equiv L(t)\rho_t , \ t \geq 0$$

(69)

where the dissipative part $L_D(t)$ is computed according to the formulas (65,67) with the Hamiltonian $H_S$ replaced by its temporal value $H_S(t)$. We can now formulate the I-st law of thermodynamics as

$$\frac{d}{dt} E(t) = \frac{d}{dt} W(t) + \frac{d}{dt} Q(t)$$

(70)

where $E(t) = \text{Tr}(\rho_t H_S(t))$ is an internal energy of $S$, $W(t) = \int_0^t \text{Tr}(\rho_s \frac{d}{ds} H_S(s)) ds$ is the work performed on $S$ by external forces and $Q(t) = \int_0^t \text{Tr}([\frac{d}{ds} \rho_s] H_S(s)) ds$ is the heat supplied to $S$ by $R$ [28,39].

In order to illustrate the second law of thermodynamics we use the relative entropy for a pair of density matrices $\rho, \sigma$

$$S(\rho|\sigma) = \text{Tr}(\rho \ln \rho - \rho \ln \sigma)$$

(71)

and the following inequality valid for any trace preserving completely positive map $\Lambda$ [37]

$$S(\rho|\sigma) \geq S(\Lambda \rho | \Lambda \sigma) .$$

(72)

For the time evolution governed by the generator $L(t)$ (eq.(69)) which possesses a temporal stationary state $L(t)\rho_{eq}(t) = 0$ , $\rho_{eq}(t) = Z^{-1} \exp\{-\beta H_S(t)\}$

(73)

the inequality (72) implies the following form of the second law of thermodynamics for open systems

$$\frac{d}{dt} S(\rho_t) = \sigma[\rho_t] + \frac{1}{T} \frac{dQ}{dt} .$$

(74)
where $\sigma[\rho_1] \geq 0$ is an entropy production and the second term describes the entropy exchainge with the heat baths. The formula (74) can be easily generalized to the case of open system coupled to several heat baths at different temperatures [28,40].

The presented derivation of the three fundamental laws of thermodynamics has been possible within the assumptions of weak coupling between $S$ to $R$ and the adiabatic change of external forces. Beyond this regime, even the unique definitions of the fundamental thermodyamic notions are not obvious. One should mention that the deviations from the thermodynamical behaviour for strongly coupled quantum systems attracted, recently, attention of the scientific community [41].

4. Low density limit

Another situation which justifies the use of MME is an open system $S$ with the discrete spectrum Hamiltonian $H_S = \sum_k \epsilon_k |k> < k|$ interacting with a dilute gas. The rigorous results can be found in [33,36] while here we present a heuristic approach. Consider first an abstract formulation of the impact approximation for the scattering problem given by the Hamiltonian $H = H_0 + V$. Starting with the identity

$$U_t = e^{-itH_0} \left( 1 + \int_0^t e^{isH_0} V e^{-isH_0} ds \right) = e^{-itH_0} \left( 1 + \int_0^t e^{isH_0} V e^{-isH_0} ds \right)$$

we replace $e^{-itH_0} e^{isH_0}$ by $\Omega_+ = \lim_{s \to \infty} e^{-itH_0} e^{isH_0}$ what makes sense for $t >> \tau_{coll}$ where $\tau_{coll}$ is a typical collision time for the discussed model. Hence we have

$$U_t \approx e^{-itH_0} \left( 1 + \int_0^t e^{isH_0} V \Omega_+ e^{-isH_0} ds \right)$$

and instead of the transition map (56) we obtain its low density counterpart

$$\rho \rightarrow \int_0^t ds_1 \int_0^t ds_2 \text{Tr}_R \left( T(s_1) \rho \otimes \omega_R T(s_2) \right)$$

where $T(s) = e^{isH_0} T e^{-isH_0}$ and $T = V \Omega_+$. In the next step we obtain a transition map similar to that derived in the weak coupling limit by averaging over the Hamiltonian evolution of $S$ and eliminating the non-resonant oscillating terms. Take a single particle of the bath being in a state described by the density matrix

$$\omega_R = \ell^{-3} \int_{\mathbb{R}^3} d^3 p \rho(p) |p>> |p|, <p|p'|>> = \delta(p - p')$$

normalized in a cube $\ell^3$ and diagonal in the momentum representation. Putting $H = H_S + \int_{\mathbb{R}^3} d^3 p \epsilon p |p>> |p|$ we obtain from (77) and for $t >> \tau_{coll}, \tau_H$ the final form of the transition map which commutes with Hamiltonian evolution

$$\rho \rightarrow t \ell^{-3} \sum_\omega \int_{\mathbb{R}^3} d^3 p \int_{\mathbb{R}^3} d^3 p' G(p) \pi \delta(E_{p'} - E_p + \omega) T_\omega(p,p') \rho T_\omega^*(p,p')$$

where

$$T_\omega(p,p') = \sum_{k,l: \epsilon_k - \epsilon_l = \omega} <k,p'|T|l,p> |k>> |l>$$

The transition map (79) corresponds to a single-particle scattering during the time interval $t$. Because in the volume $\ell^3$ we have $N$ particles the low density approximation implies additive effect producing the factor $\nu = N/\ell^3$ (instead of $\ell^{-3}$) which remains finite in the thermodynamical limit. Therefore, the final form of the MME valid under the conditions

$$\tau_H << \tau_S, \tau_{coll} << \tau_S$$

is the following

$$\frac{d}{dt} \rho(t) = -i[H_S, \rho(t)] + \nu \pi \sum_\omega \int_{\mathbb{R}^3} d^3 p d^3 p' G(p) \delta(E_{p'} - E_p + \omega) \left( [T_\omega(p,p'), \rho(t) T_\omega^*(p,p')] + [T_\omega(p,p'), \rho(t) T_\omega^*(p,p')] \right)$$
Similarly to the weak coupling limit the rigorous derivation of MME (82) involves the limit procedure \( \nu \to 0 \) for the interaction picture version of the reduced dynamics with the rescaled time \( \tau = \nu t \) [36].

It is not difficult to show that the MME (82) has similar properties to MME (65). Namely, the diagonal elements of \( \rho_t \) evolve independently of the off-diagonal ones, for the equilibrium momentum distribution of scatterers \( G(p) \sim \exp(-\beta E_p) \) the Gibbs state \( \rho_{eq} \sim \exp(-\beta H_S) \) is stationary and under natural conditions ergodic. The discussion of the Section III.C.3 can be applied also for inhomogeneous in time versions of MME (82).

5. Application to Bloch-Boltzmann equation

The MME (82) can be a starting point for the heuristic derivation of the Bloch-Boltzmann equation (36)[19]. The active atom with finite number of internal levels can be put into a finite box to take an advantage of the discrete spectrum of its momentum and kinetic energy operators. To such a discretized system of an active atom we can apply the derivation of the previous section. As an initial state we choose a quasi-diagonal density matrix

\[
\rho = \sum_v \rho(v) |v><v| \tag{83}
\]

with respect to the orthonormal velocity basis \( \{|v>\} \). Under some reasonable conditions the quasi-diagonal density matrices remains quasi-diagonal during the time evolution and finally we can go with the size of the box to infinite to obtain continuous velocity spectrum. The final result of this procedure which involves also the transition to the center of motion reference frame is the Bloch-Boltzmann equation (36)(37) with (we put here \( \hbar \) for readers convenience)

\[
H_S = \sum_{j=1}^{n} \epsilon_j |j><j|, \quad [H_S, S_a] = \omega_a S_a, \quad a = 1, 2, ..., n^2 \tag{84}
\]

\[
K_{ab}(v;v') = (2\pi)^4 \hbar^2 \mu^{-3} N_p \delta_{\omega_a,\omega_b} \int_{\mathbb{R}^3} d^3 v_r \int_{\mathbb{R}^3} d^3 v'_r \delta^3(v - v' - \frac{\mu}{m} (v_r - v'_r)) \delta\left( \frac{\mu}{2} (v_r^2 - v'_r^2) + \hbar \omega_a \right) W(v' - v_r) T_a(v_r, v'_r) T_b(v_r, v'_r) \tag{85}
\]

where \( v_r, v'_r \) denote relative velocities, \( W(v) \) is the equilibrium velocity distributions of perturbers, \( m \) is a mass of an active atom, \( \mu \) is a reduced mass of an "active atom - perturber" system, \( N_p \) is a density of perturbers and the functions \( T_a(\cdot, \cdot) \) are related to the \( T \)-matrix calculated in the center of motion reference frame by the following expression

\[
\sum_a T_a(v_r, v'_r) S_a = \sum_{j,j'=1}^{n} <v_r,j|T|v'_r,j'> |j><j'|. \tag{86}
\]

Due to the presence of Kronecker’s delta \( \delta_{\omega_a,\omega_b} \) in (85) the matrix \( K_{ab}(v;v') \) is positively defined as demanded by the conditions (37). One should mention that the obtained Bloch-Boltzmann differs from the existing ones which generally do not preserve positivity of \( \rho(v) \) [18].

D. Problems and pitfalls

The derivations of the MME presented in the previous sections are based on certain assumption concerning the decay of correlations in the environment, separation of energy levels of the open systems and the magnitude of the coupling constant or the density of perturbers. These conditions are formulated in terms of relations between the different time scales (42), (51), (63), (81). Now, we discuss briefly some of them and refer to the important physical situations beyond the presented scheme stressing the related difficulties and misconceptions.
1. Memory effects

The most demanding condition for the lack of memory of the reservoir is an inequality (58) which allows the white noise Ansatz $R_{kl}(t) \simeq \tilde{R}_{kl}(0) \delta(t)$. It means that the spectral density matrix $\tilde{R}_{kl}(\omega)$ is weakly dependent on $\omega$ in the relevant energy region. Such an assumption essentially contradicts the KMS condition (68) what is the source of the so-called thermal quantum memory characterized by the time scale $\tau_T = T^{-1}$.

Another difficulty with the assumption of memoryless reservoir can be illustrated by a model of 2-level atom coupled to the quantum electromagnetic field at the vacuum state ($T = 0$). Putting in eq.(52) the standard "dipolar electric field" interaction one obtains

$$R(t) \sim \frac{1}{(t + i\omega_c^{-1})^4}, \quad \tilde{R}(\omega) \sim \omega^3 e^{-\omega/\omega_c}$$

where $\omega_c$ is a cut-off frequency assumed to be larger than any energy scale relevant for this model. The decay of reservoir's correlations is powerlike and does not possess any natural time scale. Moreover, the correlation function is singular at the origin and $\tilde{R}(0) = 0$ for the removed cut-off ($\omega_c \to \infty$). Fortunately, in the weak coupling regime, the Markovian behaviour can be restored on the coarse-grained time scale determined by $\tau_S$ - spontaneous emission time. This is due to the averaging effect of fast Hamiltonian oscillations which allow to replace $R(t)$ by $R(t)e^{i\omega t}$ - the function which effectively acts like $\tilde{R}(\omega) \delta(t)$ under the integral in (57). The situation is different when $H_S$ is replaced by a time-dependent Hamiltonian and/or collective effect for multi-atomic systems are relevant. Namely, that fast variations of the Hamiltonian introduce high frequency contributions increasing the decay rates (see eq.(87)) and even a system of two atoms possesses degenerated energy levels for which averaging effect described above does not apply. All that implies serious limitations on the use of Markovian approximation in the context of controlled quantum open systems, the problem which is crucial for quantum information processing [42].

2. Decoherence vs. dissipation

The dynamics of an isolated quantum system is governed by its Hamiltonian $H_S$ and is characterized by two fundamental features: initial pure states remain pure, the average energy is a constant of motion. On the contrary, for an open quantum system $S$ interacting with a quantum environment $R$ which starts its joint evolution from the product state, the entangled states of $S + R$ are developed in the course of time what lead to the appearance of reduced mixed states of $S$ and the energy exchange between $S$ and $R$. The first phenomenon is called decoherence and the second one dissipation. Although decoherence and dissipation are usually present at the same time, model calculations show that for large quantum systems approaching the border between quantum and classical worlds decoherence acts on a much faster time scale than dissipation [43,44,17]. As decoherence seems to be a more important agent in the context of quantum measurement theory and quantum information processing [9] it is convenient to discuss models describing pure decoherence often called dephasing which is not accompanied by the energy exchange.

The pure decoherence is described by the models with Hamiltonians (43) satisfying the condition $[H_S^0, S_k] = 0$ what implies the same condition for the renormalized Hamiltonian $[H_S, S_k] = 0$ for all $k$. In Markovian approximations the decoherence rates are proportional to $\tilde{R}_{kl}(0)$ (see (59,60) and (65-67)) which is typically zero for the systems linearly coupled to bosonic fields. This is the case for electromagnetic interaction (87), the same result holds for linear coupling to phonons. In a general case one can formulate the following "no-go theorem" for pure decoherence:

For quantum open systems linearly coupled to bosonic reservoirs decoherence is always accompanied by dissipation.

The "physical proof" is rather simple. Any irreversible decoherence must be related to an irreversible change in the environment. In the case of linear coupling to bosonic field (48) this change can be realized only by emission or absorption of a boson - the process which changes energy of an open system as well. Obviously, in the case of scattering process governed by the bilinear interaction Hamiltonian (49) we can alter other quantum numbers of the environment’s state (e.g. its momentum) keeping the energy of $S$ conserved (elastic scattering).

One can easily find in the literature the models of dephasing based on the linear coupling to bosonic field which are essentially variations of the so-called Caldeira-Leggett model [45-47]. To explain this apparent contradiction with our "no-go theorem" consider the simplest version of the spin - boson model defined by the Hamiltonian (here $H_S \equiv 0$)

$$H_{SR} = \lambda \sigma_3 \otimes \int_0^\infty d\omega [\tilde{f}(\omega)a(\omega) + \tilde{f}(\omega)a^+(\omega)] + \int_0^\infty d\omega \omega a^+(\omega)a(\omega)$$

(88)
acting on the Hilbert space

\[ H_{SR} = C^2 \otimes F_B(L^2[0, \infty)) \equiv F_B(L^2[0, \infty)) \oplus F_B(L^2[0, \infty)) \tag{89} \]

where \( F_B(L^2[0, \infty)) \) is a bosonic Fock space over a single-particle Hilbert space \( L^2[0, \infty) \) and \([a(\omega), a^*(\omega')] = \delta(\omega - \omega')\). The unitary Weyl operator \( U_g \) acting on fields operators as

\[ U_g a(\omega) U_g^* = a(\omega) + g(\omega) \tag{90} \]

exists if and only if \( g \in L^2(0, \infty) \). Putting

\[ g(\omega) = \lambda \omega^{-1} f(\omega) \tag{91} \]

we can diagonalize \( H_{SR} \) (88)

\[ U_g H_{SR} U^*_g = \int_0^\infty d\omega \omega a^*(\omega)a(\omega) + \text{const.} \tag{92} \]

where

\[ U_g = \begin{pmatrix} U_g & 0 \\ 0 & U_{-g} \end{pmatrix} \tag{93} \]

The ground states subspace of the diagonalized Hamiltonian (92) is spanned by the vectors \( |1 > \otimes |\Omega >, |2 > \otimes |\Omega > \) and therefore the corresponding degenerated ground states of \( H_{SR} \) are given by

\[ |1 > \otimes |\phi[-g] >, |1 > \otimes |\phi[g] >, \text{where } |\phi[g] > = U_g |\Omega >, g(\omega) = \lambda \omega^{-1} f(\omega). \] \tag{94} \]

The vectors \( |\phi[\pm g] > \) are coherent states in \( F_B(L^2[0, \infty)) \) and

\[ < \phi[-g], \phi[g] > = \exp{-2\|g\|^2}. \tag{95} \]

Assume now that we would like to describe dephasing of our spin using the model given by (88). Then we should have \( \mathcal{R}(0) = \lambda^2 |f(0)|^2 > 0 \) what implies due to (91) that the function \( g(\omega) \) is not square integrable i.e. \( \|g\| = \infty \). The same divergence appears for any "ohmic" or "subohmic" coupling \( |f(\omega)|^2 \sim \omega^s \) around 0 with \( 0 \leq s \leq 1 \). It follows that the diagonalizing transformation of a bosonic field (90) cannot be implemented by the unitary operator on the Fock space and therefore the formal expression (88) does not define a meaningful bounded from above Hamiltonian. It means that for an arbitrary coupling constant \( \lambda \) the model given by (88) is neither nonphysical or cannot describe exponential (Markovian) dephasing. In a less mathematical language the large value of \( \|g\| \) due either to a large coupling constant or to a large integral \( \int_0^\infty d\omega \omega^{-2} |f(\omega)|^2 \) makes the coherent states \( |\phi[\pm g] > \) corresponding to a "cloud" and the vacuum \( |\Omega > \) almost orthogonal. As a consequence the standard choice of the initial state as a product state \( \rho \otimes |\Omega > < \Omega | \) is inappropriate and impossible to prepare. The proper initial state should have a support spanned by the "dressed" ground states (94). The computed lost of coherence for the former choice of the initial state is therefore unphysical and describes the spurious process of a "cloud formation". Again the problem of a proper decomposition of the total system into open system and environment such that the effective interaction between them is weak, is crucial for the physical interpretation of the obtained results.

One should mention that from the mathematical point of view the above example illustrates the subtle problem of nonequivalent representations of canonical commutation relations for systems with infinite number of degrees of freedom [48].

3. Open systems with continuous spectrum

In the derivations of MME based on the weak coupling or low density limits the discretness of \( H_S \) spectrum plays a crucial role. The averaging over Hamiltonian oscillations justifies the Markovian approximation on the coarse-grained time scale and the canceling of non-resonant terms is a necessary condition to preserve complete positivity of the QDS. This interplay between the self-evolution of \( S \) and the interaction with \( R \) produces the desired properties of QDS like for instance the relaxation to a proper equilibrium state for \( R \) being a heat bath.
However, there are important examples of open systems with continuous spectrum of $H_S$, the most studied is a quantum Brownian particle. For simplicity, we discuss first the case of Brownian motion in one-dimensional space. The most frequently used MME for this case is the so-called Caldeira-Leggett equation \cite{47} of the form
\begin{equation}
\frac{d}{dt} \rho_t = -i[H_S, \rho_t] - i\gamma [X, \{P, \rho_t\}] - 2M\gamma T[X, [X, \rho_t]]
\end{equation}
where $X, P$ are position and momentum operators, $H_S = P^2/2M + V(X)$, $\gamma$ is a friction constant and $M$- mass of the Brownian particle. $V(X)$ is a generic potential which can produce both continuous and discrete parts of the energy spectrum.

The MME (96) possesses the following well-known drawbacks:
1) the solution of (96) does not preserve positivity of the density matrix,
2) the Gibbs state (perhaps unnormalized) $\sim \exp\{-H_S/T\}$ is not its stationary state.

The first drawback can be cured by adding the term $-\gamma(8MT)^{-1}[P, [P, \rho_t]]$ which allows to write the corrected MME in a standard form \cite{13,14}. However the dissipative part of this new generator corresponds to a damped harmonic oscillator one \cite{27} (with $\gamma_1 = 0$) and the Hamiltonian part gains the correction $\sim (XP + PX)$ with a rather unclear physical interpretation.

In author’s opinion the above difficulties have its source in the underlying Hamiltonian model for $S + R$ system, the so-called Caldeira-Leggett model, which is essentially a non-zero temperature version of the model \cite{88} with $\sigma_3$ replaced by the operator $X$ and the ”forbidden” ohmic choice of $\int f(\omega)^2\sim \omega$ around zero. In other words according to the ”no-go theorem” the equation (96) which in the extreme heavy particle limit ($M \rightarrow \infty$) describes pure decoherence cannot be derived from a physically admissible model with linear coupling to the bosonic reservoir.

It seems, that for a continuous spectrum of $H_S$ the lack of a natural time scale provided by the Hamiltonian evolution makes impossible to find a single MME which accurately describes all relevant stages of the evolution of $S$ \cite{49}. We do not mean here the well-known and expected deviations from the Markovian (exponential) behaviour for very short times typically $\sim \omega_c^{-1}$ ($\omega_c$ - cut-off frequency) and very long ones (due to the boundness from below of the Hamiltonian of $R$). In the simplest case of a Brownian particle in the free space described by the center of mass position $X$ and the total momentum $P$ the situation can be summarized in a following way.

The proper model of an environment should involve interactions of the type \cite{49} describing scattering process with particles of the medium. Beside the direct collisions with atoms, molecules, photons etc. the other ”bilinear” processes are possible within this model like for instance absorption of a foton followed by the excitation of the internal degrees of freedom of the Brownian particle and the time-reversed process \cite{17}.

The following different but approximatively Markovian stages of the evolution can be singled out:

1) Pure decoherence stage, when the decay of macroscopically distinguishable quantum superpositions into mixed states dominates over energy thermalization. For the low density medium and/or small Brownian particle this stage is well-described by the eq.(35) on the time scale determined by $\tau_{dec} = (\int d^3k n(k))^{-1}$. For dense media or/and large particle $\tau_{dec}$ can be comparable or shorter than the already mentioned time scale $\omega_c^{-1}$ what demands a different theoretical treatment \cite{50}.

2) Thermalization stage, when the density matrix of the Brownian particle written in momentum representation is close to diagonal i.e. $\rho_t(p, p')$ differs essentially from zero for $|p - p'| \leq \sqrt{2MT}$. The detailed analysis of this regime and the manifest standard form of MME which depends on the so-called dynamic structure factor characterizing the environment are presented in \cite{51}.

Another completely different situation where the continuous spectrum of $H_S$ appears is the theory of many-body open systems. An ensemble of interacting quantum spins coupled to an infinite heat bath and described in the thermodynamic limit is a perfect example. The mathematical formalism used in this context to construct proper MME, difficulties and partial solutions of the problems are discussed in \cite{52}.

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