



Dynamics of Open Quantum Systems—Markovian Semigroups and Beyond

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Abstract: The idea of an open quantum system was introduced in the 1950s as a response to the problems encountered in areas such as nuclear magnetic resonance and the decay of unstable atoms. Nowadays, dynamical models of open quantum systems have become essential components in many applications of quantum mechanics. This paper provides an overview of the fundamental concepts of open quantum systems. All underlying definitions, algebraic methods and crucial theorems are presented. In particular, dynamical semigroups with corresponding time-independent generators are characterized. Furthermore, evolution models that induce memory effects are discussed. Finally, measures of non-Markovianity are recapped and interpreted from a perspective of physical relevance.

Keywords: open quantum systems; quantum master equations; Markovian semigroups; time-local generators; non-Markovian dynamics; information flow; quantum non-Markovianity; nonlocality in time; memory effects

1. Introduction

In physics, time belongs to fundamental quantities (base quantities), and it is used to derive other elementary concepts such as motion, velocity or energy. Physicists have always been interested in finding the most accurate ways to describe how physical systems change over time. To achieve this goal, we need mathematical laws, for example, kinetic equations that include the information about the dynamics and interaction between the system and its environment. The equations differ in the level of accuracy and in the kind of system they describe. All the approaches to dynamics of physical systems can be most generally divided into two groups—classical and quantum. Since the paper focuses on open quantum systems, more attention is given to the evolution in the microscopic scale. However, for historical accuracy, a brief recap of the dynamics of classical systems is also presented.

The idea of an open quantum system, i.e., a physical system of interest interacting with some environment, was introduced in the 1950s as a response to the problems encountered in areas such as nuclear magnetic resonance and the decay of unstable atoms. It became evident that, in order to properly describe such physical processes, one had to take into account the influence of the environment on the system in question. In a pioneering work on this topic, A.G. Redfield applied for nuclear magnetic resonance spectroscopy, a master equation that describes the time evolution of a quantum system weakly coupled to an environment [1]. In another paper, R. Haag and D. Kastler, working within the quantum field theory, introduced maps (originally in the article called operations) that can be used to describe a quantum system influenced by an external intervention [2]. Their approach was later developed by K.-E. Hellwig and K. Kraus [3,4].

In the 1970s, there was a rapid expansion of the theory of open systems. There were numerous groundbreaking works that laid the foundations for the theory of open quantum systems in its present shape, see, for example, Refs. [5–7]. In this paper, we revise the remarkable results achieved in 1976 on the structure of the generator of quantum dynamical



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Copyright: © 2022 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). semigroups [8,9] as well as the findings related to the properties of completely positive and trace-preserving (CPTP) maps [10,11]. In addition, we discuss selected concepts of non-Markovian dynamics, which involves a revival of genuine quantum properties due to backflows of information. Lastly, we analyze the nonlocal approach to quantum dynamics that is based on the Nakajima-Zwanzig equation. Throughout the paper, we pay special attention to the mathematical rigor and physical interpretations of the presented content.

2. Classical Dynamical Semigroups

Let us start with introducing a probability space (probability triple), which consists of three elements—a sample space Ω (assumed to be a finite or countable set of all possible outcomes), a set of events Θ and the assignment of probabilities to the events (probability function) μ . Altogether the probability space shall be denoted by: (Ω, Θ, μ) . A probability measure μ assigned to an element $\omega_i \in \Omega$ shall be denoted by p_i . The set of quantities p_i for $i = 1, ..., N \leq \infty$ defined by the assignment:

$$\Omega \ni \omega_i \to p_i = \mu(\omega_i) \in [0, 1],\tag{1}$$

can be treated as coordinates of a certain vector, denoted by \mathbf{p} , which belongs to an *N*-dimensional real vector space \mathcal{X} with a specific basis. The coordinates of the vector \mathbf{p} satisfy two conditions:

$$p_i \ge 0$$
 for $i = 1, ..., N$ and $\sum_{i=1}^N p_i = 1.$ (2)

Henceforth, a vector **p** that satisfies the two conditions (2) shall be called a probability vector. Such terminology is commonly used in the literature on the probability theory (e.g., [12,13]). The set of all probability measures defined on the measurable space (Ω, Θ) will be denoted by $\Gamma(\Omega)$. This set is a convex subset of the set of all measures assigned to the measurable space (Ω, Θ) . The relation (1) allows one to consider probability measures as a specific kind of vectors in space \mathcal{X} .

Let us consider, as an example, a case such that dim $\mathcal{X} < \infty$, which means that the set of elementary events Ω is finite. Then, the map (1) allows one to identify the probability measures defined on (Ω, Θ) with the elements of the set

$$\Gamma(\Omega) := \left\{ \mathbf{p} = (p_1, \dots, p_N) : p_i \ge 0, \quad \sum_{i=1}^N p_i = 1 \right\},$$
(3)

i.e., with the elements of the (N - 1)-dimensional simplex in the space $\mathcal{X} = \mathbb{R}^N$. The vertices of the simplex are determined by the vectors: $\mathbf{p}_1^0 = [1, 0, \dots, 0]$ and $\mathbf{p}_N^0 = [0, 0, \dots, 1]$.

Let S denote a physical system such that one can associate with it a finite or countable set of all possible physical states of the system in question. According to general schemes of the probability theory, the events from the set are treated as elements of some abstract Boole's σ -algebra (see more, for example, in Ref. [14]). Bearing in mind Stone's theorem [15], which claims that every abstract Boole's σ -algebra is isomorphic with some algebra of selected subset of Ω , we shall use the definitions.

Definition 1 (Classical stochastic system). The system S is called an N-level classical stochastic system if its state at any time instant $t \in R^1_+$ is determined by a probability distribution $p(t) \in \Gamma(\Omega)$. The set $\Gamma(\Omega) \subsetneq \mathcal{X}$ is called the state space of the classical stochastic system S.

Definition 2 (Pure and mixed states). Let p_k^0 denote a vector such that $p_k = 1$ and $p_j = 0$ for $j \neq k$. Then, the states of a classical stochastic system expressed by the probability vectors of the form p_k^0 (for k = 1, ..., N) shall be called pure states of the system S. Other states are called mixed.

Definition 3 (Norm in \mathcal{X}). In the space \mathcal{X} (dim $\mathcal{X} < \infty$), one defines a norm in the following way:

$$||x||_1 := |x_1| + \ldots + |x_N|.$$
(4)

The space \mathcal{X} with the norm introduced as in (4) is denoted by l_1^N .

Definition 4 (Infinite-dimensional linear space). Analogously, l_1^{∞} denotes the infinite-dimensional linear space composed of all sequences $x = \{x_i\}_{i=1}^{\infty}$ such that

$$||x||_1 := \sum_{i=1}^{\infty} |x_i| < \infty.$$

One can rewrite the formula (3) for the state space of an *N*-level classical stochastic system S by using the definition of the norm introduced in (4)

$$\Gamma(\Omega) := \{ \mathbf{p} \in l_1^N : \ \mathbf{p} \ge 0, \ ||\mathbf{p}||_1 = 1 \}.$$
(5)

A natural problem that appears at this moment is how to describe linear changes of the state of an *N*-level classical physical system S. Mathematically speaking, one needs to consider a linear operator Φ acting in the space l_1^N such that

$$\Phi: \ \Gamma(\Omega) \to \Gamma(\Omega)$$

i.e., an operator that transforms states into states. The answer to this problem is rather trivial—the desired kind of operator in its matrix representation is a left stochastic matrix, which means that the entries are nonnegative real numbers and the elements in each column sum to one

$$\Phi(i,j) \ge 0, \qquad \sum_{i=1}^{N} \Phi(i,j) = 1, \quad \text{for} \quad i,j = 1, \dots, N < \infty.$$
 (6)

The matrix representation of Φ is called the Markov matrix, and its elements are interpreted as transition probabilities. Any operator Φ that satisfies the conditions from (6) can be considered a classical channel, which maps one state into another. However, from the point of view of system dynamics, it is desirable to be able to determine a continuous set of all state vectors for a certain physical system, i.e., one needs to find the trajectory of the state vector within the state space. Such a trajectory shall be denoted by $\{\mathbf{p}(t), t \in \mathbb{R}^1_+\}$.

Mathematically speaking, in order to analyze the evolution of a classical system, it is essential to introduce a family of classical maps that depends on one real parameter, denoted by *t*, which in physics can be understood as time. In both classical and quantum cases, the theory of dynamical semigroups constitutes the foundation for such analysis, c.f. Refs. [5,16]. The definition of a classical dynamical semigroup can be found in many books. Here, we follow the definition from Ref. [17]. Let us first denote the lowest dimensional linear space which contains the state space by $l_1(\Omega)$ (i.e., $l_1(\Omega) = l_1^N$ or $l_1(\Omega) = l_1^\infty$). Then, we can formulate the following definition.

Definition 5 (Classical dynamical semigroup). A family $\{\Phi(t), t \in R^1_+\}$ of linear maps such that $\Phi(t) : l_1(\Omega) \to l_1(\Omega)$ shall be called a classical dynamical semigroup of a physical system S if

1.
$$\Phi(t): \Gamma(\Omega) \to \Gamma(\Omega) \quad \forall t \in \mathbb{R}^{1}_{+},$$

2. $\Phi(t)\Phi(s) = \Phi(t+s) \quad \forall t, s \in \mathbb{R}^{1}_{+},$
3. $\lim_{t \to 0} \Phi(t) = \mathbb{I},$

where \mathbb{I} denotes the identity operator in $l_1(\Omega)$. The limit which appears in the last equation should be understood as a limit in terms of the norm $||.||_1$ in $l_1(\Omega)$.

For the sake of physical relevance, we distinguish a specific kind of classical dynamical semigroup—a regular dynamical semigroup (sometimes called a proper dynamical semigroup).

Definition 6 (Regular (proper) dynamical semigroup). A classical dynamical semigroup $\{\Phi(t), t \in R^1_+\}$ containing maps such that $\Phi(t) : l_1(\Omega) \to l_1(\Omega)$ shall be called a regular (proper) dynamical semigroup, if there exists a linear operator

$$L: \quad l_1(\Omega) \to l_1(\Omega)$$

such that

$$\Phi(t) = \exp(Lt)$$

for all $t \in \mathbb{R}^1_+$. The operator L is referred to as the generator of the semigroup $\{\Phi(t), t \in \mathbb{R}^1_+\}$.

The distinguished position of classical dynamical semigroups can be explained by the following reasoning. If $\{\Phi(t), t \in \mathbb{R}^1_+\}$ denotes a regular dynamical semigroup and $L: l_1(\Omega) \to l_1(\Omega)$ is its generator, then for all $\mathbf{p} \in l_1(\Omega)$, the following relation is satisfied

$$\frac{d}{dt}\{\Phi(t)\mathbf{p}\}=L[\Phi(t)\mathbf{p}].$$

Moreover, by substituting $\mathbf{p}(t) = \Phi(t)\mathbf{p}$ for all $t \ge 0$, one obtains an equation that demonstrates how the probability vector **p** changes with time

$$\frac{d\mathbf{p}(t)}{dt} = L[\mathbf{p}(t)] \qquad \forall t \in R^1_+.$$
(7)

Equations of the form (7) are commonly called master equations (sometimes also kinetic equations), and they are widely used to describe the different forms of evolution of physical, chemical, or biological systems.

In other words, one can say that every trajectory $\{\mathbf{p}(t), t \in R^1_+\}$ that is defined by a regular dynamical semigroup $\{\Phi(t), t \in \mathbb{R}^1_+\}$ is a solution of a master Equation (7). Additionally, if one makes an assumption concerning the initial state vector: $\mathbf{p}(0) \in \Gamma(\Omega)$, then for all $t \in R^1_+$:

$$R^1_+ \ni t \to \mathbf{p}(t) \in \Gamma(\Omega)$$

which means that the trajectory determined by the semigroup does not leave the state space, i.e.,

$$\{\mathbf{p}(t), t \in R^1_+\} \subset \Gamma(\Omega)$$

Finally, one may ask a question concerning the conditions that should be satisfied by the generator of a regular dynamical semigroup. The answer to this problem was found in 1931 by A. Kolmogorov; see more in Ref. [18].

Theorem 1 (Kolmogorov 1931). The equations of the form:

$$\frac{dp_i(t)}{dt} = \sum_{j=1}^N L_{ij}p_j(t)$$

are kinetic equations if and only if the matrix entries of the generator L satisfy the three following conditions:

- 1.
- $\begin{array}{ll} L_{ii} \leq 0 & for \ i = 1, \dots, N, \\ L_{ij} \geq 0 & for \ i \neq j \ and \ i, j = 1, \dots, N, \\ \sum_{i=1}^{N} L_{ij} = 0 & for \ j = 1, \dots, N. \end{array}$ 2.
- 3.

The result proved by A. Kolmogorov provides the sufficient criteria that have to be satisfied by a linear operator $L : l_1(\Omega) \rightarrow l_1(\Omega)$ to generate a legitimate model of classical evolution. In the context of continuous-time Markov processes, the generator L is termed a transition rate matrix [19]. If one takes a legitimate generator of evolution, then for every initial state vector $\mathbf{p}(0) \in \Gamma(\Omega)$, the trajectory $\{\mathbf{p}(t), t \in R^1_+\}$ determined by the master Equation (7) lies within the state space $\Gamma(\Omega)$.

From a modern perspective, the original representation of the transition rate matrix is not the most general. For systems with multiple steady states, the generator can be represented as a block diagonal matrix. Then, a single block may or may not satisfy the third condition from Theorem 1. More specifically, it is not satisfied when a steady state does note reside in the block of *L*. This concept, which is known as open system symmetries, was studied in the quantum context but also remains relevant to classical stochastic systems, see more in Ref. [20].

3. Quantum Dynamical Semigroups

Quantum dynamical semigroups appear to be a natural method to describe the dynamics of quantum systems. However, within the quantum theory, they are only considered one of the possible approaches to this problem (other influential techniques related to quantum dynamics involve the Redfield equation, the path integral formulation, the Fokker–Planck equation, or the hierarchical equations of motion). Let us first revise the necessary notation and symbols. We consider an open quantum system S. The Hilbert space associated with the system shall be denoted by \mathcal{H} (sometimes, in order to emphasize that the space is related to the system, it is denoted by \mathcal{H}_S). The corresponding well-defined scalar product shall be denoted by $\langle \psi | \phi \rangle$ for any vectors $|\psi\rangle$, $|\phi\rangle \in \mathcal{H}$.

Throughout the paper, the Dirac notation is used, which means that $\langle \psi |$ refers to the conjugate transpose (the Hermitian conjugate or the Hermitian transpose) of $|\psi\rangle$. Thus, $\langle \psi |$ is obtained by taking the transpose of $|\psi\rangle$ and then taking the complex conjugate of each entry. The Hermitian conjugate shall be denoted by a star, which is common in linear algebra, i.e., $|\psi\rangle^* = \langle \psi |$.

If one assumes that the Hilbert space is finite-dimensional, one may introduce an orthonormal basis $\{|x_i\rangle\}_{i=1}^d$ satisfying $\langle x_i|x_j\rangle = \delta_{ij}$, where $d = \dim \mathcal{H}$. In the present paper, we do not consider infinite-dimensional Hilbert spaces.

Throughout the paper, we use the following notations [21]:

- 1. $B(\mathcal{H})$ shall refer to the complex vector space of all linear operators on \mathcal{H} with an operator norm for $A \in B(\mathcal{H})$ defined by $||A||_{HS} := \sqrt{\text{Tr}(A^*A)}$, where, by A^* , we mean the Hermitian transpose of A (this norm is often referred to as the Hilbert–Schmidt norm, and for this reason, there is an abbreviation "HS" in the subscript of the norm);
- 2. $B_*(\mathcal{H})$ shall refer to the real Banach space of self-adjoint (Hermitian) operators on \mathcal{H} , i.e., $B_*(\mathcal{H}) := \{A : \mathcal{H} \to \mathcal{H}, A^* = A\};$
- 3. $V^+(\mathcal{H})$ shall refer to the cone of all positive semi-definite operators within $B(\mathcal{H})$ (an operator *A* is called positive semi-definite (denoted by $A \ge 0$) if and only if $\langle \phi | A | \phi \rangle \ge 0$ for all $| \phi \rangle \in \mathcal{H}$), i.e., $V^+(\mathcal{H}) = \{A : \mathcal{H} \to \mathcal{H}, A \ge 0\}$;
- 4. $T(\mathcal{H})$ shall refer to the vector space of trace class operators (A is said to be a trace class operator if $||A||_{\text{Tr}} := \text{Tr}\sqrt{AA^*} < \infty$). If dim $\mathcal{H} = d < \infty$, then the vector spaces $B(\mathcal{H})$ and $T(\mathcal{H})$ are isomorphic. However, they are not identical, because the norm is defined in different ways.

Then, we make a distinction between pure and mixed quantum states. A pure quantum state is represented by a normalized complex vector $|\phi\rangle$ belonging to the Hilbert space \mathcal{H} or, alternatively, by a projector onto a one-dimensional subspace, i.e., $\Pi := |\phi\rangle\langle\phi|$.

A mixed quantum state, if the associated Hilbert space \mathcal{H} has a fixed basis, is represented by a density matrix—a Hermitian nonnegative matrix with unit trace—which can be generally decomposed in the form:

$$\rho := \sum_{\kappa} \lambda_{\kappa} |\phi_{\kappa}\rangle \langle \phi_{\kappa}|, \tag{8}$$

where $\langle \phi_{\kappa} | \phi_{\eta} \rangle = \delta_{\kappa \eta}$, $\lambda_{\kappa} \ge 0$ and $\sum_{\kappa} \lambda_{\kappa} = 1$. The formalism of density operators was introduced in 1927 by John von Neumann [22] and, simultaneously, by Lev Landau [23], however, the latter did it less rigorously.

According to the fundamental assumptions of quantum mechanics, the density matrix contains all achievable information about the state of a physical system. Therefore, the problem of state identification, i.e., the density matrix reconstruction from experimental data, has been relevant to many modern areas of quantum theory; as can be seen in Refs. [24,25].

Bearing in mind the general decomposition of any density operator, one can write the definition of a set that contains all physically legitimate quantum states:

$$S(\mathcal{H}) := \{ \rho : \mathcal{H} \to \mathcal{H}, \quad \rho \ge 0, \quad \rho^* = \rho, \quad \operatorname{Tr} \rho = 1 \}, \tag{9}$$

which shall be called the set of states.

An important property of the set of states is convexity, which means that every convex combination of density operators belongs to $S(\mathcal{H})$, i.e., if one takes nonnegative numbers $a_1, \ldots, a_M \geq 0$ such that $\sum_{i=1}^M a_i = 1$ and density operators $\sigma_1, \ldots, \sigma_M \in S(\mathcal{H})$, then $\sum_{i=1}^{M} a_i \sigma_i$ also belongs to the set of states.

Another useful property of density operators claims that $\gamma \equiv \text{Tr } \rho^2 \leq 1$ for all $\rho \in S(\mathcal{H})$. We know that max $\gamma = 1$ if and only if ρ is a pure state. On the other hand, min $\gamma = 1/d$ for a maximally mixed state. For given density operators, this property can be used to distinguish pure states from mixed ones. In a more general sense, γ is a measure on quantum states, giving information on how much a state is mixed. The quantity γ is commonly called the purity [26].

Geometrically speaking, one can imagine that the condition $Tr\rho = 1$, which we impose on quantum states, cuts the cone of all positive semi-definite operators $V^+(\mathcal{H})$ so that the dimension of the $S(\mathcal{H})$ is lowered by 1.

In order to describe how quantum systems change over time, we need to determine the properties of a one-parameter family of linear operators $\Phi(t)$ such that for all $t \in R^+_+$ quantum states are mapped into quantum states, i.e.,

$$\Phi(t): S(\mathcal{H}) \to S(\mathcal{H}).$$

The conditions that the family of maps $\{\Phi(t), t \in R^1_+\}$ should satisfy to guarantee a legitimate physical evolution can be combined together in a definition of a quantum dynamical semigroup [5,17,27].

Definition 7 (Quantum dynamical semigroup). A one-parameter family $\{\Phi(t), t \in \mathbb{R}^1_+\}$ of linear maps such that $\Phi(t) : B_*(\mathcal{H}) \to B_*(\mathcal{H})$ shall be called a quantum dynamical semigroup of a physical system S if

1.

$$\begin{split} \Phi(t): \ V^+(\mathcal{H}) &\to V^+(\mathcal{H}) \quad \forall \ t \in R^1_+; \\ ||\Phi(t)[\rho]||_{\mathrm{Tr}} = ||\rho||_{\mathrm{Tr}} \quad \forall \ \rho \in V^+(\mathcal{H}) \quad and \quad \forall \ t \in R^1_+; \end{split}$$
2.

3.
$$\Phi(t)\Phi(s) = \Phi(t+s) \quad \forall t, s \in \mathbb{R}^1_+;$$

4.
$$\lim_{t \to 0} \Phi(t) = \mathbb{I},$$

where I denotes the identity operator in $B_*(\mathcal{H})$. The limit which appears in the last equation should *be understood as a limit in terms of the norm* $||.||_{Tr}$

The conditions enumerated in Definition 7 are very natural from the physical point of view. Points 1. and 2. ensure that, for all $t \in R^1_+$, the operator $\Phi(t)$ transforms a quantum state into another state, i.e., $\Phi(t) : S(\mathcal{H}) \to S(\mathcal{H})$. Condition 3. guarantees that the one-parameter family $\{\Phi(t), t \in R^1_+\}$ constitutes a semigroup. Finally, the last condition ensures that for any $Q \in B_*(\mathcal{H})$, the following equation is satisfied: $\lim_{t \to 0} \operatorname{Tr}(Q(\Phi(t)[\rho] - \rho)) = 0.$

Nevertheless, in spite of its physical relevance, one needs to look at the problem differently to be able to use the mathematical properties of quantum semigroups. In Ref. [5], it was proven that the conditions listed in Definition 7 are equivalent to the following set of terms.

Definition 8 (Kossakowski 1972). A one-parameter family $\{\Phi(t), t \in R^1_+\}$ of linear maps such that $\Phi(t) : B_*(\mathcal{H}) \to B_*(\mathcal{H})$ constitutes a quantum dynamical semigroup of a physical system S if

1. $\operatorname{Tr}(\Phi(t)[\rho]) = \operatorname{Tr} \rho \quad \forall \rho \in B_*(\mathcal{H}) \quad and \quad \forall t \in R^1_+;$ 2. $||\Phi(t)[\rho]||_{\operatorname{Tr}} = ||\rho||_{\operatorname{Tr}} \quad \forall \rho \in B_*(\mathcal{H}) \quad and \quad \forall t \in R^1_+;$ 3. $\Phi(t)\Phi(s) = \Phi(t+s) \quad \forall t, s \in R^1_+;$ 4. $\lim_{t \to 0} \Phi(t) = \mathbb{I}.$

The key difference between the two definitions of a quantum dynamical semigroup is that the conditions 1. and 2. of Definition 8 refer to the vector space $B_*(\mathcal{H})$, not like in the case of Definition 7 only to the cone $V^+(\mathcal{H})$.

By applying the Hille–Yosida theorem (see, for example, Refs. [28,29]) to a quantum semigroup { $\Phi(t)$, $t \in R^1_+$ }, one can affirm that there exists a linear operator \mathbb{L} : $B_*(\mathcal{H}) \to B_*(\mathcal{H})$ such that

$$\frac{d}{dt}\{(\Phi(t)[\rho]\} = \mathbb{L}[\Phi(t)[\rho]],\tag{10}$$

for all $\rho \in D(\mathbb{L})$, where $D(\mathbb{L})$ denotes the domain of the operator \mathbb{L} (the domain lies within the vector space $B_*(\mathcal{H})$).

In case of quantum dynamical semigroups, we also distinguish a class of regular dynamical semigroups [30].

Definition 9 (Regular quantum dynamical semigroup). A quantum dynamical semigroup $\{\Phi(t), t \in R^1_+\}$, which consists of maps such that $\Phi(t) : B_*(\mathcal{H}) \to B_*(\mathcal{H})$, shall be called a regular dynamical semigroup if there exists a linear bounded operator:

$$\mathbb{L}: B_*(\mathcal{H}) \to B_*(\mathcal{H})$$

such that

$$\Phi(t) = \exp(\mathbb{L}t)$$

for all $t \in R^1_+$. The entire vector space $B_*(\mathcal{H})$ is the domain of the operator \mathbb{L} .

For a *d*-level quantum system (dim $\mathcal{H} < \infty$), every dynamical semigroup is regular (because every linear operator from $B_*(\mathcal{H})$ is bounded). In other words, if dim $\mathcal{H} < \infty$, every family of maps { $\Phi(t)$, $t \in R^1_+$ } ($\Phi(t) : B_*(\mathcal{H}) \to B_*(\mathcal{H})$) that satisfies the conditions enumerated in Definition 8 can be expressed in the exponential form: $\Phi(t) = \exp(\mathbb{L}t)$ for $t \in R^1_+$, where the operator $\mathbb{L} : B_*(\mathcal{H}) \to B_*(\mathcal{H})$ is called the generator of evolution.

By substituting $\rho(t) \equiv \Phi(t)[\rho]$ to the differential Equation (10), one obtains the master equation in a succinct form:

$$\frac{d\rho(t)}{dt} = \mathbb{L}[\rho(t)],\tag{11}$$

where the initial condition states: $\rho(0) = \rho$. Sometimes, a master equation of the form (11) is called the quantum Liouville equation, and the generator \mathbb{L} is referred to as the Liouville operator.

8 of 24

4. Positive and Completely Positive Maps

The concept of completely positive maps was introduced by Stinespring in 1955 [31]. However, the motivation behind Stinespring's work was purely mathematical because it was a part of the research into *C**-algebras, and there was no proposal to apply this idea to quantum physics. The problem of the proper description of changes in a quantum system due to external intervention was investigated in the 1960s in the works of R. Haag and D. Kastler, as well as K.-E. Hellwig and K. Kraus—see, for example, Refs. [2–4]. In one of the very first articles on open quantum systems [2], the authors mathematically introduced maps (originally called operations) that can be applied to describe the interactions between a given physical system and other external systems. The concept of positive and completely positive maps was later developed by Kraus and described in papers such as Refs. [10,11].

Nowadays, positive and completely positive maps are widely applied in many areas of physics—quantum computing and quantum information [26]), quantum entanglement detection [32,33] and the evolution of quantum systems [34–37].

To describe the changes of a quantum state, one needs to analyze linear operators Λ (sometimes called superoperators) such that $\Lambda : B(\mathcal{H}) \to B(\mathcal{H})$. The action of every operator of this kind can be written in the following way (this decomposition is not unique and only holds for finite-dimensional spaces; see, for example, Ref. [38]):

$$\Delta[X] = \sum_{i=1}^{\eta} \lambda_i \, A_i X B_i, \tag{12}$$

where $\lambda_i \in \mathbb{C}$ and $A_i, B_i \in B(\mathcal{H})$ for all $i = 1, ..., \eta$. Now let us define specific kinds of maps.

Definition 10 (Hermiticity preserving maps). Λ preserves Hermiticity \iff

$$\forall X \in B(\mathcal{H}) \quad (\Lambda[X])^* = \Lambda[X^*]. \tag{13}$$

Properties of such maps which preserve Hermiticity are often analyzed in the quantum theory. One may prove that, in the case of Hermiticity-preserving maps, the general decomposition of Λ as from (12) can be transformed into:

$$\Lambda[X] = \sum_{i=1}^{N} \alpha_i A_i X A_i^*, \tag{14}$$

where $\alpha_i \in \mathbb{R}$ and $A_i \in B(\mathcal{H})$ for all i = 1, ..., N.

Definition 11 (Trace-preserving maps). Λ preserves trace \iff

$$\forall X \in B(\mathcal{H}) \quad \operatorname{Tr}(\Lambda[X]) = \operatorname{Tr}(X).$$
(15)

Definition 12 (Identity-preserving maps). Λ preserves identity \iff

Λ

$$\Lambda[\mathbb{I}] = \mathbb{I}. \tag{16}$$

An identity-preserving map is termed unital.

Definition 13 (Positive map). Λ *is called positive* \iff

$$\forall X \in V^+(\mathcal{H}) \quad \Lambda[X] \ge 0. \tag{17}$$

According to Definition 13, determining whether a map Λ is positive would require checking an infinite number of conditions.

Definition 14 (*k*-positivity). Λ is called *k*-positive if and only if the map $\mathbb{I}_k \otimes \Lambda$ acting:

$$\mathbb{I}_k \otimes \Lambda : \mathbb{M}_k(\mathbb{C}) \otimes B(\mathcal{H}) \to \mathbb{M}_k(\mathbb{C}) \otimes B(\mathcal{H})$$
(18)

is positive.

In (18), the symbol $\mathbb{M}_k(\mathbb{C})$ denotes the space of all $k \times k$ complex matrices and \mathbb{I}_k denotes the identity operator in $\mathbb{M}_k(\mathbb{C})$.

Remark 1 (k^{th} **amplification**). The map $\mathbb{I}_k \otimes \Lambda$ is called the k^{th} amplification of the map Λ .

Remark 2. If a map Λ is k-positive, it is also (k - 1)-positive, (k - 2)-positive, (k - 3)-positive, ..., 2-positive.

The concept of *k*-positivity is necessary to introduce the definition of completely positive maps (often written CP maps for short).

Definition 15 (Complete positivity). A map $\Lambda : B(\mathcal{H}) \to B(\mathcal{H})$ is called completely positive *(CP) if and only if the map* $\mathbb{I}_k \otimes \Lambda$ *is positive for all* $k \in \mathbb{N}$ *. In other words,* Λ *is completely positive, when it is k-positive for* k = 1, 2, ...

Remark 3. A map that satisfies the condition for complete positivity (Definition 15) and is tracepreserving (Definition 11) is called a quantum channel. Completely positive and trace-preserving maps are often abbreviated to CPTP maps.

Thankfully, in practice, one does not have to check the positivity of an infinite number of maps $\mathbb{I}_k \otimes \Lambda$ (k = 1, 2, 3, ...) in order to judge whether Λ is CP or not. A result obtained by Choi gives a better understanding of CP maps [39].

Theorem 2 (Choi theorem [39]). If dim $\mathcal{H} = d$, then Λ is CP if and only if Λ is d-positive.

If \mathcal{P}_k denotes the convex set of all *k*-positive maps, one can formulate the following chain of inclusions:

CP maps
$$\equiv \mathcal{P}_d \subset \mathcal{P}_{d-1} \subset \cdots \subset \mathcal{P}_2 \subset \mathcal{P}_1 \equiv \text{positive maps}$$

As an example, one can consider the transposition $\mathcal{T}_d : \mathbb{M}_d(\mathbb{C}) \to \mathbb{M}_d(\mathbb{C})$, which is standard algebraic operation, i.e., $\mathcal{T}_d[X] = X^T$. This operator does not change the eigenvalues of X, which implies that $X^T \ge 0$ for any $X \ge 0$. One can also notice that \mathcal{T}_d is unital and preserves the trace. However, if we consider $\mathbb{I}_2 \otimes \mathcal{T}_2$, it turns out that this map is not positive in $\mathbb{M}_4(\mathbb{C})$. This means that the map \mathcal{T}_d is not CP.

Another example relates to the reduction map $\mathcal{R}_d : \mathbb{M}_d(\mathbb{C}) \to \mathbb{M}_d(\mathbb{C})$ that is defined as

$$\mathcal{R}_d[X] := rac{1}{d-1}(\mathbb{I}_d\operatorname{Tr} X - X).$$

It can be demonstrated that this map is positive [40]. In addition, it preserves the trace and identity. However, if one again considers $\mathbb{I}_2 \otimes \mathcal{R}_2$, it can be proved that this map is not positive in $\mathbb{M}_4(\mathbb{C})$, which implies that \mathcal{R}_d is not CP.

From Theorem 2, one can observe that, in order to verify whether Λ is CP, it is sufficient to investigate the positivity of only one map, namely: $\mathbb{I}_d \otimes \Lambda$. However, as has already been stated, according to Definition 13, checking the positivity, in general, requires verifying an infinite number of conditions. Fortunately, thanks to the Choi-Jamiołkowski isomorphism (channel-state duality), the verification of complete positivity is made easier [41].

Theorem 3 (Choi-Jamiołkowski theorem). A linear map $\Lambda : B(\mathcal{H}) \to B(\mathcal{H})$, where dim $\mathcal{H} = d$, is CP if and only if:

$$(\mathbb{I}_d \otimes \Lambda)[P_d^+] \ge 0, \tag{19}$$

where P_d^+ denotes the projector onto the maximally entangled state $P_d^+ = \frac{1}{d} \sum_{i,j=1}^d E_{ij} \otimes E_{ij}$ (the symbol E_{ij} relates to a matrix with *ij*-th entry equal to 1 and others equal zero).

Theorem 3 can be considered a milestone result for modern quantum theory, because it states that in order to prove that a map Λ is CP, one needs to demonstrate that $(\mathbb{I}_d \otimes \Lambda)$ is positive only on one operator—the projector onto maximally entangled state P_d^+ .

Another commonly used theorem concerning CP maps is the so-called Kraus representation [11].

Theorem 4 (Kraus representation). A linear map $\Lambda : B(\mathcal{H}) \to B(\mathcal{H})$ is completely positive if and only if for any $X \in B(\mathcal{H})$:

$$\Lambda[X] = \sum_{\alpha} K_{\alpha} X K_{\alpha}^{*}, \qquad (20)$$

where $K_{\alpha} \in B(\mathcal{H})$.

Although the formula (20) is called the Kraus representation and the operators K_{α} are usually referred to as the Kraus operators, it was not introduced by Kraus. The above decomposition of CP maps appeared already in 1961 in Ref. [42]. Furthermore, it is worth mentioning that the Kraus representation is non-unique.

As was already mentioned, a CPTP map is called a quantum channel. Based on the Kraus representation, one may write the following definition of the quantum channel.

Definition 16 (Quantum channel). A linear map $\Lambda : B(\mathcal{H}) \to B(\mathcal{H})$ is a quantum channel if and only if:

$$\forall \quad X \in B(\mathcal{H}) \qquad \Lambda[X] = \sum_{\alpha} K_{\alpha} X K_{\alpha}^{*}$$

and

$$\sum_{\alpha} K_{\alpha}^* K_{\alpha} = \mathbb{I}_d.$$
⁽²¹⁾

The condition in (21) ensures that the map Λ preserves the trace of X. Typical examples of quantum channels studied within quantum information theory include bit flip and phase flip, depolarizing, amplitude damping, and phase damping channels [26].

In order to describe the changes of a quantum system over time, one needs to introduce time-dependent CPTP maps Λ_t . Maps that are legitimate from the physical point of view are called dynamical maps.

Definition 17 (Dynamical map). A one-parameter continuous family of maps $\{\Lambda_t, t \in R^1_+\}$ such that $\Lambda_t : B(\mathcal{H}) \to B(\mathcal{H})$ constitutes a dynamical map if and only if:

- 1. Λ_t is completely positive for all $t \in R^1_+$;
- 2. Λ_t is trace-preserving for all $t \in R^1_+$;
- 3. $\Lambda_0 = \mathbb{I}$.

The last condition in the definition of a dynamical map is natural, because if a family of maps $\{\Lambda_t, t \in R^1_+\}$ is used to describe the evolution of a density operator, it has to satisfy the initial condition $\Lambda_0[\rho(0)] = \rho(0)$.

If the initial density operator $\rho(0)$ is known, a dynamical map determines the trajectory of a quantum state because it defines the assignment:

$$R^1_+ \ni t \to \rho(t) := \Lambda_t[\rho(0)]. \tag{22}$$

There exists a general decomposition of a dynamical map that allows one to describe any evolution of the density matrix: $\Lambda_{(t_1,t_0)}$: $\rho(t_0) \rightarrow \rho(t_1)$ [43,44].

Theorem 5 (Salgado et al. [43] and Tong et al. [44]). Any kind of time evolution of a quantum state $\rho(t_0)$ can always be written in the form

$$\rho(t_1) \equiv \Lambda_{(t_1, t_0)} \left[\rho(t_0) \right] = \sum_{\alpha} K_{\alpha}(t_1, t_0, \rho) \,\rho(t_0) \, K^*_{\alpha}(t_1, t_0, \rho), \tag{23}$$

where the operators $K_{\alpha}(t_1, t_0, \rho)$ depend on the state ρ at time t_0 .

The significance of Theorem 5 relates to its generality. For any density operator, regardless of the initial condition and the path of its evolution in the state space, the time evolution of the state can always be described in terms of an operator-sum representation (Kraus representation). However, we would rather have mathematical formalism that describes a physical process independently of the state it acts upon. In this way, we can obtain a universal dynamical map that can be imposed on any initial state. Furthermore, such an approach gives a precise description of the interactions by means of operators. This leads to another definition [35].

Definition 18 (Universal dynamical map (UDM)). A dynamical map is termed universal if it is independent of the state it acts upon. The most general form of a UDM is given by

$$\rho(t_1) \equiv \Lambda^{UDM}_{(t_1,t_0)} \left[\rho(t_0) \right] = \sum_{\alpha} K_{\alpha}(t_1,t_0) \, \rho(t_0) \, K^*_{\alpha}(t_1,t_0)$$

with a condition

$$\sum_{\alpha} K_{\alpha}^*(t_1, t_0) K_{\alpha}(t_1, t_0) = \mathbb{I}_{\alpha}$$

that guarantees $\text{Tr}(\rho(t_1)) = 1$ for any initial state $\rho(t_0)$.

Theorem 5 and Definition 18 demonstrate how powerful the Kraus representation is. Not only does it apply to transformations of quantum states, but also to the time-continuous evolution of the density matrix.

5. Dynamics of Closed Quantum Systems

The dynamics of closed quantum systems is a well-known subject that has been thoroughly described in numerous publications. This section on closed systems was written based on four high-profile publications—Chapter 3.1. of Ref. [45], Chapter 2 of Ref. [46], Chapter 2 of Ref. [35], and Chapters 2 and 8 of Ref. [26].

A quantum system is said to be closed (or isolated) if it does not interact with another physical system, i.e., the system in question does not interchange information with another system. Mathematically, the description of such systems is relatively simple. However, in a laboratory, it is impossible to achieve perfectly isolated systems. Nevertheless, the dynamics of closed systems is a necessary step to understanding open quantum systems.

The problem of quantum systems evolution lies at the very foundations of quantum mechanics. The first approach to describe the changes over time of a physical system was proposed in 1926 by E. Schrödinger, who derived an evolution equation which was later named after the author—the Schrödinger Equation [47]. A state vector $|\psi(t)\rangle \in \mathcal{H}$, which contains information about a certain closed physical system in the pure state, evolves in time according to the equation:

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle,$$
 (24)

where $i^2 = -1$, \hbar denotes the Dirac constant (the Planck constant divided by 2π) and $H \in B_*(\mathcal{H})$ is a fixed Hermitian operator known as the Hamiltonian of the closed system.

The exact value of the constant \hbar is not important in the most presented considerations. Thus, we shall put $\hbar = 1$.

One can easily observe that, in order to possess the complete knowledge about changes over time in a closed system, it is necessary and sufficient to have the Hamiltonian of the system. However, in general, determining the Hamiltonian that describes a particular system is a very difficult task, which requires much data from an experiment.

One of the key features of the Schrödinger equation is the fact that it does not change the norm of the states, which can be easily proved:

$$\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = \left(\frac{d\langle\psi(t)|}{dt}\right)|\psi(t)\rangle + \langle\psi(t)|\left(\frac{d|\psi(t)\rangle}{dt}\right) = i\langle\psi(t)|H^*|\psi(t)\rangle - i\langle\psi(t)|H|\psi(t)\rangle = 0,$$
(25)

because the Hamiltonian belongs to the space of self-adjoined operators, i.e., $H^* = H$.

Since the Schrödinger equation, as was shown in (25), cannot change the norm of a state vector, the solution of the equation for a finite dimensional system has to be given by a unitary operator:

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle,\tag{26}$$

where $U(t,t_0)U^*(t,t_0) = U^*(t,t_0)U(t,t_0) = \mathbb{I} \iff U^{-1}(t,t_0) = U^*(t,t_0).$

The fact that a unitary operator constitutes a map that does not change the norm (i.e., a norm-preserving map) can be manifested in a simple way. Let us assume that the solution of the Schrödinger equation is given by a map $|\psi(t)\rangle = V(t, t_0)|\psi(t_0)\rangle$ and we demand that this map has to be norm-preserving. Then, we can obtain:

$$\begin{aligned} \langle \psi(t) | \psi(t) \rangle &= \langle \psi(t_0) | V^*(t, t_0) V(t, t_0) | \psi(t_0) \rangle \\ \langle \psi(t_0) | \psi(t_0) \rangle &\longleftrightarrow \\ V^*(t, t_0) V(t, t_0) &= \mathbb{I} \iff V^*(t, t_0) = V^{-1}(t, t_0) \end{aligned}$$

and one can confirm that the only kind of map which guarantees norm-preserving is unitary. Naturally, the unitary operator which appears in (26) is the exponential form of the Hamiltonian from (24), i.e.,

$$U(t,t_0) = \exp(-iH(t-t_0)).$$

In the case of mixed states of closed (isolated) quantum systems, one has to use the von Neumann equation in order to describe the dynamics of the system. Any mixed state can be considered a statistical mixture of pure states $|\psi_k(t)\rangle$ (each of them evolves according to the Schrödinger equation) with nonnegative weights λ_k . Therefore, the evolution equation for any density operator of a closed system $\rho(t) := \sum_k \lambda_k |\psi_k(t)\rangle \langle \psi_k(t)|$ can be quickly derived on the basis of the Schrödinger equation:

$$\begin{aligned} \frac{d\rho(t)}{dt} &= \sum_{k} \lambda_{k} \frac{d|\psi_{k}(t)\rangle \langle \psi_{k}(t)|}{dt} = \sum_{k} \lambda_{k} \left(\frac{d|\psi_{k}(t)\rangle}{dt} \langle \psi_{k}(t)| + |\psi_{k}(t)\rangle \frac{d\langle \psi_{k}(t)|}{dt} \right) = \\ &= \sum_{k} \lambda_{k} (-iH|\psi_{k}(t)\rangle \langle \psi_{k}(t)| + i|\psi_{k}(t)\rangle \langle \psi_{k}(t)|H) = \\ &= -i\sum_{k} \lambda_{k} [H, |\psi_{k}(t)\rangle \langle \psi_{k}(t)|] = -i[H, \sum_{k} \lambda_{k} |\psi_{k}(t)\rangle \langle \psi_{k}(t)|] = \\ &= -i[H, \rho(t)], \end{aligned}$$

where [A, B] denotes the commutator of A and B, i.e., [A, B] := AB - BA.

The solution of the von Neumann equation can also be easily obtained on the basis of the Schrödinger equation:

$$|\psi_k(t)\rangle = U(t,t_0)|\psi_k(t_0)\rangle \iff |\psi_k(t)\rangle\langle\psi_k(t)| = U(t,t_0)|\psi_k(t_0)\rangle\langle\psi_k(t_0)|U^*(t,t_0),$$

which gives the formula for $\rho(t)$:

$$\rho(t) = \sum_{k} \lambda_{k} U(t, t_{0}) |\psi_{k}(t_{0})\rangle \langle\psi_{k}(t_{0})| U^{*}(t, t_{0}) = U(t, t_{0})\rho(t_{0}) U^{*}(t, t_{0}).$$
(27)

One can notice that the unitary evolution (27) resulting from the von Neumann equation is an example of UDM. The evolution of closed systems is described by only one time-dependent operator $U(t, t_0)$. Naturally, this kind of dynamics is CP since the map is given in the Kraus form. Furthermore, the unitary operator property, $U^{-1}(t, t_0) = U^*(t, t_0)$, is equivalent to the condition for trace-preserving maps (21).

6. Evolution of Open Quantum Systems

An open quantum system, on the contrary to closed systems, interacts with the other system called the environment. The dynamics of open quantum systems has been the subject of extensive research in recent years. There have been many approaches to study open quantum systems' evolution. In spite of a large number of publications revealing new results on open systems' dynamics, there are still many unsolved problems.

In this section, we revise selected concepts on the evolution of open quantum systems. The content is divided into three parts. First, in Section 6.1, a brief summary of the reduced dynamics is given, which is essential to understand the idea of open systems. Then, in Section 6.2, we present the most important results on local in time approach to open systems' evolution. The results are accompanied by selected algebraic tools needed for solving problems related to this scope (such as the method of vectorization). Finally, in Section 6.3, a short review on the nonlocal in time approach is presented.

6.1. Reduced Dynamics of Open Quantum Systems Evolution

In this section, we shall revise the concept of reduced dynamics. Since there are two physical parts, coupled and interacting with each other, in this case, one needs to consider two Hilbert spaces— H_S associated with the system of interest S and H_E corresponding to the environment \mathcal{E} .

The physical system of interest shall be described by a density matrix $\rho(t) \in S(\mathcal{H}_S)$ and the environment by a quantum state $\rho_E(t) \in S(\mathcal{H}_E)$.

Apparently, the evolution of the total system $S + \mathcal{E}$ (described by the density matrix $\rho_{SE}(t)$) is unitary and determined by a Hamiltonian that can be expressed as:

$$H = H_S \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E + H_{int}, \tag{28}$$

where H_S , $\mathbb{I}_S : \mathcal{H}_S \to \mathcal{H}_S$, H_E , $\mathbb{I}_E : \mathcal{H}_E \to \mathcal{H}_E$, and $H_{int} : \mathcal{H}_S \otimes \mathcal{H}_E \to \mathcal{H}_S \otimes \mathcal{H}_E$.

Under two approximations, one is able to derive a computable formula for the evolution of the quantum system of interest.

- 1. First crucial assumption claims that the coupling between the system and the environment is weak and, therefore, the quantum state of the environment does not change in time and can be simply denoted by ρ_E .
- 2. The other important assumption claims that there is no initial correlation between the system and its environment, i.e., $\rho_{SE}(0) = \rho(0) \otimes \rho_E$.

Based on these two assumptions, the dynamical map given by means of the partial trace over the environmental degrees of freedom has the form

$$\rho(t) = \operatorname{Tr}_E[U(t)\,\rho(0) \otimes \rho_E \,U^*(t)] \tag{29}$$

where $U(t) : \mathcal{H}_S \otimes \mathcal{H}_E \to \mathcal{H}_S \otimes \mathcal{H}_E$ is the unitary operator that governs the evolution of the total system $S + \mathcal{E}$, i.e., $U(t) = \exp(-iHt)$, where the Hamiltonian *H* is defined in (28). The symbol Tr_E denotes partial trace over \mathcal{H}_E .

Evolution of an open quantum system can also be described by a dynamical map Λ_t (see Definition 17 and the assignment (22)).

One can notice that there are two alternative approaches to open quantum dynamics (One can find more in Section 3.2. of Ref. [35]).

- 1. One may consider the initial state of environment+system $\rho_{SE}(0) = \rho(0) \otimes \rho_E$ and apply to it unitary evolution. In order to obtain the evolution of the system in question, it is required to perform the partial trace as indicated in (29) to eliminate the degrees of freedom related to the environment.
- 2. One may reduce the initial environment+system state and apply a dynamical map only to the system of interest (see (22)).

Both approaches are equivalent because every dynamical map induced from the unitary evolution of an extended system with the initial condition $\rho_{SE}(0) = \rho(0) \otimes \rho_E$ is a UDM and vice versa [35].

The assumption that the system and the environment are initially in a separable tensor product state is intrinsically linked with the property of complete positivity of dynamical maps. In a wide variety of realistic situations, it is justified to expect that we have sufficient control over the system to guarantee that it is decoupled from its environment. However, in more general treatment, there may be some initial correlations between the system and its bath. In such circumstances, one cannot rely on CP maps to model the evolution of the system. It turns out that the reduced dynamics of S is described by maps that are not CP; see more in Refs. [48,49].

Furthermore, there have been multiple attempts to go beyond the weak-coupling approximation. For example, fourth-order quantum master equations can be derived for a general system Hamiltonian, which provides corrections in the intermediate system-bath coupling regime [50]. Other approaches to extend the dynamics beyond the weak-coupling limit involve: improved Dyson series expansion [51], hierarchical equations of motion [52], quasi-adiabatic propagator path integral [53], or the correlation picture approach [54].

6.2. Local in Time Approach to Open Quantum Systems Evolution

In the second half of the XX century, there was a scientific debate on a generalization of the von Neumann equation in order to make it applicable to open quantum systems. As a result of this dispute, two articles have been published in 1976—one written by V. Gorini and A. Kossakowski, and G. Sudarshan [8] and the other by G. Lindblad [9]. Both articles contain very similar results and interestingly, they were submitted and published almost simultaneously. These articles are considered milestones for the development of the theory of open quantum systems.

In a historical article Ref. [55], the authors established the sequence of events. In 1972, A. Kossakowski published a landmark article with an axiomatic definition of dynamical semigroups [5]. Between 26 March and 6 April 1973, V. Gorini attended the conference *Foundations of quantum mechanics and ordered linear spaces*, where he learned about the concept of complete positivity from K. Kraus and E. Stormer. Both V. Gorini and A. Kossakowski visited G. Sudarshan from September to December 1974 at the University of Texas in Austin. G. Lindblad preferred to work individually. In December 1974, he participated in the Symposium on Mathematical Physics, organized by R. Ingarden in Toruń. Lindblad's seminar at the conference was devoted to quantum dynamical semigroups. He used the conference to announce his most recent results for the first time (see the letter from Lindblad published in [55]). In January 1975, V. Gorini visited Lindblad in Stockholm, and both researchers compared the results on quantum dynamical semigroups which were obtained independently. First, on 19 March 1975, V. Gorini, A. Kossakowski, and G. Sudarshan submitted their manuscript, which was published in May 1976 [8]. On 7 April 1975, G. Lindblad submitted their paper, which appeared in June 1976 [9].

Although two articles on the generators of quantum dynamical semigroups were published in 1976, the discovery was not immediately disseminated within the community. In 1984, T. Banks, L. Susskind, and M.E. Peskin published a work entitled "Difficulties for the Evolution of Pure States Into Mixed States", in which they investigated "the general properties of evolution equations for ρ ". They arrived at the solution that closely resembles

the results by V. Gorini et al. and G. Lindblad, but their methods suggest that they had not known the papers from 1976 [56].

The main result published in the articles [8,9] relates to the properties of the generator \mathbb{L} of a quantum dynamical semigroup. However, neither of the articles gives a general answer regarding what conditions a generator \mathbb{L} should satisfy so that the solution of the equation

$$\dot{\Lambda}_t = \mathbb{L}[\Lambda_t] \tag{30}$$

determines a quantum dynamical semigroup Λ_t . Although in both cases the problem was narrowed, it does not decrease the significance of the results and its applicability to physical problems.

On the basis of [8], one can formulate the following theorem.

Theorem 6 (GKS generator). A linear operator $\mathbb{L} : \mathbb{M}_d(\mathbb{C}) \to \mathbb{M}_d(\mathbb{C})$ generates a completely positive semigroup if it can be represented in the form:

$$\mathbb{L}[\rho(t)] = -i[H,\rho(t)] + \frac{1}{2} \sum_{p,q=1}^{d^2-1} \alpha_{pq} \Big([F_p \,\rho(t), F_q^*] + [F_p,\rho(t) \, F_q^*] \Big), \tag{31}$$

where $H^* = H$, $\operatorname{Tr} H = 0$, $\operatorname{Tr} F_p = 0$ (for $p = 1, \ldots, d^2 - 1$), $\operatorname{Tr}(F_p F_q^*) = \delta_{pq}$ (for $p, q = 1, \ldots, d^2 - 1$) and the elements α_{pq} constitute a positive semi-definite matrix. Moreover, the symbol $\mathbb{M}_d(\mathbb{C})$ denotes the algebra of $d \times d$ complex matrices.

The matrix $[\alpha_{pq}]$ is sometimes called the Kossakowski matrix. If the basis $\{F_j\}$ is given, one needs to know the Kossakowski matrix and the Hamiltonian in order to determine the trajectory of a quantum state.

Lindblad used a different approach—he worked in the Heisenberg picture at the level of $B(\mathcal{H})$, and by applying different methods, he obtained a result which can be presented in the following theorem [9].

Theorem 7 (Lindblad generator). A linear operator \mathbb{L}^* : $\mathbb{M}_d(\mathbb{C}) \to \mathbb{M}_d(\mathbb{C})$ generates a completely positive semigroup if and only if it has the following form:

$$\mathbb{L}^{*}[X] = i[H, X] + \frac{1}{2} \sum_{k=1}^{d^{2}-1} \gamma_{i} \left(V_{k}^{*} X V_{k} - \frac{1}{2} \{ V_{k}^{*} V_{k}, X \} \right),$$
(32)

where $V_k \in B(\mathcal{H})$ and $\sum_k V_k^* X V_k \in B(\mathcal{H})$. The symbol $\{A, B\}$ denotes anticommutator, i.e., $\{A, B\} = AB + BA$. The operators V_i can be called Lindblad operators or jump operators. The coefficients γ_k are called decoherence rates and they have to satisfy $\gamma_k \ge 0$ for all k.

One should bear in mind that the generator \mathbb{L}^* in the Heisenberg picture can be easily transformed into the generator \mathbb{L} in the Schrödinger picture:

$$\mathbb{L}[\rho(t)] = -i[H,\rho(t)] + \sum_{k=1}^{d^2-1} \gamma_i \bigg(V_k \rho(t) V_k^* - \frac{1}{2} \{ V_k^* V_k, \rho(t) \} \bigg),$$
(33)

The equation $\frac{d\rho(t)}{dt} = \mathbb{L}[\rho(t)]$ with the generator given by (31) or (33) is the most general type of Markovian and time-homogeneous master equation which preserves trace and positivity. Both forms of the generator of evolution are equivalent because every positive semi-definite matrix $[\alpha_{pq}]$ can be diagonalized so that the result matrix has only nonnegative elements on the main diagonal. Therefore, hereafter in this paper, any generator of evolution of the form either (31) or (33) shall be called a GKSL generator (Gorini–Kossakowski–Sudarshan–Lindblad generator). The derivation of the GKSL master equation and its properties can be found in Ref. [57].

In the 1970s, V.A. Franke was also searching for the most general linear transformations of the density matrices of an open quantum system that preserve the properties of ρ and do not generate negative probabilities [58]. His paper was submitted on 6 October 1975 and published in May 1976. The results obtained by V.A. Franke are close to Refs. [8,9]. Therefore, some authors name the generator of a quantum dynamical semigroup as: Franke–Gorini–Kossakowski–Lindblad–Sudarshan (FGKLS), see for example, Ref. [59].

On the basis of (33), one can reformulate the definition of the generator \mathbb{L} by introducing a completely positive map Φ .

Remark 4. If one denotes

$$\Phi[\rho(t)] \equiv \sum_{k=1}^{d^2-1} \gamma_k V_k \rho(t) V_k^*,$$

then the generator \mathbb{L} can be equivalently presented in the form:

$$\mathbb{L}[\rho(t)] = -i[H,\rho(t)] + \Phi[\rho(t)] - \frac{1}{2} \{\Phi^*[\mathbb{I}_d],\rho(t)\},\tag{34}$$

where Φ is completely positive and Φ^* denotes the dual map to Φ .

Alternatively, the generator of evolution \mathbb{L} can be presented in the explicit matrix form that is obtained by employing the method of vectorization. For any matrix A, the operator vec[A] denotes a vector constructed by stacking the columns of A one underneath the other. This operation has some unique properties. In particular, to transform the generator of evolution given by (33), one applies the relation that connects vectorization with the standard matrix product and the Kronecker product [60–62]

$$\operatorname{vec}\{XYZ\} = (Z^{T} \otimes X) \operatorname{vec}\{Y\},\tag{35}$$

which holds for matrices X, Y, Z selected in such a way that the matrix product XYZ is computable.

Taking into account the relation (35), one obtains the matrix representation of the GKSL generator

$$\mathbb{L} = i(H^T \otimes \mathbb{I}_d - \mathbb{I}_d \otimes H) + \sum_{k=1}^{d^2 - 1} \gamma_k \bigg(\overline{V}_k \otimes V_k - \frac{1}{2} \mathbb{I}_d \otimes V_k^* V_k - \frac{1}{2} V_k^T \overline{V}_k \otimes \mathbb{I}_d \bigg),$$
(36)

where \overline{V}_k denotes the complex conjugate of the operator V_k . The property (36) is commonly called the Roth's column lemma. The explicit matrix form of the generator of evolution is useful in the context of quantum tomography because it allows one to determine the algebraic properties of the generator \mathbb{L} [63,64]. Furthermore, the Roth's column lemma can be useful in quantum optimal control theory (see more, for example, Ref. [65]).

Quantum dynamical semigroups are only one of the possible approaches to local-intime quantum dynamics. More generally, one should consider a master equation with a time-dependent generator \mathbb{L}_t

$$\frac{d\rho(t)}{dt} = \mathbb{L}_t[\rho(t)],\tag{37}$$

where $\mathbb{L}_t : \mathbb{M}_d(\mathbb{C}) \to \mathbb{M}_d(\mathbb{C})$ is a linear operator. The dynamics (37) can be called timeconvolutionless (TCL) master equation, and the generator \mathbb{L}_t does not have to be in the GKSL form.

Any linear operator \mathbb{L}_t can be explicitly represented in its matrix form by using the method of vectorization (bear in mind the general form of any linear operator—Equation (12)). Thus, any evolution equation with a time-dependent linear operator takes the form:

$$\operatorname{vec}\{\dot{\rho}(t)\} = \mathbb{L}_t \operatorname{vec}\{\rho(t)\},\tag{38}$$

where between \mathbb{L}_t and vec{ $\rho(t)$ } there is a standard algebraic multiplication, i.e., the column vector vec{ $\rho(t)$ } is multiplied by the matrix \mathbb{L}_t . Thus, one way of analyzing such dynamics requires investigating the algebraic properties of \mathbb{L}_t .

Alternatively, the master Equation (37) can be rewritten so that it describes how Λ_t changes over time:

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$$\Lambda_t = \mathbb{L}_t[\Lambda_t]. \tag{39}$$

Equation (39) is analogous to (30).

Apart from Equation (39), there is another formula that connects the map Λ_t with the generator \mathbb{L}_t . Let us assume that we know a certain dynamical map Λ_t that is invertible, i.e., there exists a map $\Lambda_t^{-1} : \mathbb{M}_d(\mathbb{C}) \to \mathbb{M}_d(\mathbb{C})$ such that $\Lambda_t^{-1}\Lambda_t = \Lambda_t\Lambda_t^{-1} = \mathbb{I}_d$. Then, one can write [40,66]:

$$\dot{\Lambda}_t = \dot{\Lambda}_t \Lambda_t^{-1} \Lambda_t = \mathbb{L}_t [\Lambda_t], \tag{40}$$

from which one can observe that

$$\mathbb{L}_t := \Lambda_t \Lambda_t^{-1}, \tag{41}$$

which means that, starting with a legitimate dynamical map Λ_t that is invertible, one can calculate the corresponding time-dependent generator \mathbb{L}_t . However, the inverse map Λ_t^{-1} is very difficult to construct and it does not need to be completely positive (to be precise, for a CP map Λ_t , the inverse map Λ_t^{-1} is also CP if and only if $\Lambda_t[X] = U(t) X U^*(t)$, which means that Λ_t has to be unitary).

In 1949, F. Dyson published a work, where he presented the formal solution of an explicitly time-dependent Schrödinger Equation [67]. The result was obtained by iteration and a time ordering operator that was later called, after the author, the Dyson series. Thus, the formal solution of Equation (37) can be written as follows:

$$\Lambda_t = \hat{T} \, \exp\left(\int_0^t \mathbb{L}_\tau d\tau\right),\tag{42}$$

where \hat{T} denotes the chronological product. The formula (42) can be expanded by applying the Dyson series [67]:

$$\Lambda_t = \mathbb{I}_d + \int_0^t dt_1 \mathbb{L}_{t_1} + \int_0^t dt_1 \int_0^{t_1} dt_2 \mathbb{L}_{t_1} \mathbb{L}_{t_2} + \dots,$$
(43)

provided it converges. For some specific types of time-dependent generators, the TCL master equation can be solved without the necessity of implementing the Dyson series. In particular, functionally commutative [68] and partially commutative generators [69] lead to simple dynamical maps since the \hat{T} product can be dropped out.

One might consider the following question.

What algebraic properties should a local-in-time generator \mathbb{L}_t possess in order to guarantee that Λ_t defined by the Dyson series in (43) generates a legitimate dynamical map?

Generally, the answer to this question is not known; however, there are many specific cases of the generator \mathbb{L}_t such that one can prove the map Λ_t is legitimate.

One commonly known case is a time-dependent GKSL generator [70,71]. It can be proved that the trace and Hermiticity of a density matrix are preserved by the time-dependent generator in the form:

$$\mathbb{L}_{t}[\rho(t)] = -i[H(t), \rho(t)] + \sum_{k=1}^{d^{2}-1} \gamma_{k}(t) \left(V_{k}(t) \rho(t) V_{k}^{*}(t) - \frac{1}{2} \{ V_{k}^{*}(t) V_{k}(t), \rho(t) \} \right), \quad (44)$$

where H(t) denotes a time-dependent effective Hamiltonian that accounts for the unitary evolution, and $V_k(t)$ are time-dependent Lindblad operators. The functions $\gamma_i(t)$ are called decoherence rates, and in this approach, they also depend on time.

If the relaxation rates are nonnegative functions for all time instants, i.e., $\gamma_k(t) \ge 0$ for all *k* and for any $t \ge 0$, then the generator from (44) is in the GKSL form (c.f. (33)) for each fixed $t \ge 0$. Such dynamics can be considered time-dependent Markovian, although the corresponding dynamical map Λ_t does not lead to a quantum dynamical semigroup [72].

On the other hand, if the relaxation rates are negative on some time intervals, then the generator from (44) has different properties than the GKSL generator (33). For example, it does not have to be a completely positive generator. However, some particular constructions of \mathbb{L}_t with negative decoherence rates guarantee a legitimate evolution that leads to non-Markovian effects. Such dynamics feature backflows of information from the environment to the system. However, the evolution is still local in time because there is no convolution (integral) of the open system states with a memory kernel.

Different frameworks were proposed to assess whether a given dynamical map describing a physical process could have arisen from Markovian dynamics [73]. On the level of quantum dynamical maps, the distinction between Markovian and non-Markovian evolution can be made on the basis of CP-divisibility. Let us recall the definition.

Definition 19 (**Propagator of the dynamics**). A dynamical map Λ_t can be decomposed as

$$\Lambda_t = V(t,s) \Lambda_s, \quad \text{for } t \ge s \ge 0, \tag{45}$$

where V(t,s) is termed the propagator of the dynamics. Moreover, if Λ_t^{-1} exists, then the propagator can be computed from

$$V(t,s) = \Lambda_t \circ \Lambda_s^{-1}.$$

Based on the notion of the propagator, one can define CP-divisibility.

Definition 20 (CP-divisibility). A dynamical map Λ_t is called CP-divisible if its propagator V(t,s) is CP for all $t \ge s \ge 0$.

The property of CP-divisibility is strictly connected with Markovianity, i.e., quantum evolution is Markovian if and only if the corresponding dynamical map Λ_t is CP-divisible [74,75]. For time-local generators (44), the dynamical map Λ_t is CP-divisible if and only if the relaxation rates $\gamma_k(t)$ of the generator (44) are nonnegative for all $t \ge 0$. One can verify that for dynamics governed by a GKSL generator (33), the corresponding dynamical map $\Lambda_t = \exp(\mathbb{L}t)$ is CP-divisible, which stems from the properties of a dynamical semigroup.

The property of CP-divisibility of Λ_t defines Markovian evolution. For a propagator V(t, s) that is not CP but only *k*-positive, we can define the notion of *k*-divisibility.

Definition 21 (k-divisibility). A dynamical map Λ_t is called k-divisible is and only if the corresponding propagator V(t,s) is k-positive for all $t \ge s \ge 0$.

One can notice that CP-divisible maps correspond to *d*-divisibility. To clarify the notation, let us call 1-divisible maps P-divisible. The definition of *k*-divisibility allows us to introduce a degree of non-Markovianity [76].

Definition 22 (Non-Markovianity Degree (NMD)). We say that a dynamical map Λ_t has a non-Markovianity degree $NMD[\Lambda_t] = m$ if and only if the map is (d - m)-divisible but it is not (d - m + 1)-divisible.

From the definition of NMD, one can see that for Markovian maps, $NMD[\Lambda_t] = 0$ while for P-divisible maps, which are called essentially non-Markovian, $NMD[\Lambda_t] = d$. The concept of *k*-divisibility allows us to compute a series of natural measures that quantify the departure from *k*-divisibility [76].

Definition 23 (Non-Markovianity measures). The departure from k-positivity is quantified as

 $\mathcal{M}_k[\Lambda_t] = \sup_X rac{\Sigma_k^+[X]}{|\Sigma_k^-[X]|},$

where

$$\Sigma_k^+[X] = \int_{\zeta_k(X;t)>0} \zeta_k(X;t) \, dt$$

and

$$\zeta_k(X;t) := rac{d}{dt} \| (\mathbb{I}_k \otimes \Lambda_t)[X] \|_{\mathrm{Tr}}.$$

 $\Sigma_k^-[X]$ is analogously computed by integrating over time integrals such that $\varsigma_k(X;t) < 0$. The supremum is taken over all Hermitian operators $X \in \mathbb{M}_k(\mathbb{C}) \otimes B(\mathcal{H})$.

It can be proven that $|\Sigma_k^-[X]| \ge \Sigma_k^+[X]$, which implies that $\mathcal{M}_k[\Lambda_t] \in [0, 1]$ [76]. Furthermore, one can check that for l > k, we have $\mathcal{M}_l[\Lambda_t] > \mathcal{M}_k[\Lambda_t]$, which leads to a chain of inequalities

$$0 \leq \mathcal{M}_1[\Lambda_t] \leq \ldots \leq \mathcal{M}_d[\Lambda_t] \leq 1.$$

Finally, a map Λ_t is called maximally non-Markovian if and only if $\mathcal{M}_1[\Lambda_t] = 1$, which gives $\mathcal{M}_1[\Lambda_t] = \ldots = \mathcal{M}_d[\Lambda_t] = 1$.

Markovian generators \mathbb{L}_t constitute a convex cone within the space of all legitimate local in time generators, which means that a convex combination of two Markovian generators is also Markovian, i.e., $\alpha_1 \mathbb{L}_t^{(1)} + \alpha_2 \mathbb{L}_t^{(2)}$ is Markovian for any two Markovian generators $\mathbb{L}_t^{(1)}$ and $\mathbb{L}_t^{(2)}$ and for any $\alpha_1, \alpha_2 \ge 0$.

An analogous proposition would not be true for dynamical maps, i.e., if there are two CP-divisible maps (i.e., Markovian maps) $\Lambda_t^{(1)}$ and $\Lambda_t^{(2)}$, their convex combination $\alpha_1 \Lambda_t^{(1)} + \alpha_2 \Lambda_t^{(2)}$ does not have to be CP-divisible [74]. In Ref. [77], a simple but very educational example illustrating this fact was provided. Let us consider two time-local generators:

$$\mathbb{L}^{(1)}[\rho(t)] = \frac{c}{2}(\sigma_1 \rho(t) \sigma_1 - \rho(t)) \quad \text{and} \quad \mathbb{L}^{(2)}[\rho(t)] = \frac{c}{2}(\sigma_2 \rho(t) \sigma_2 - \rho(t)), \tag{46}$$

where c > 0 and σ_1, σ_2 denote, by convention, two Pauli matrices.

Naturally, both generators are in the GKSL form, and therefore, they are CP-divisible. The dynamical maps corresponding with the generators have the following form $\Lambda_t^{(1)} = e^{t \mathbb{L}^{(1)}}$ and $\Lambda_t^{(2)} = e^{t \mathbb{L}^{(2)}}$. Let us notice that one might obtain the following convex combination of maps:

$$\Lambda_t[\rho(0)] = \frac{1}{2}\Lambda_t^{(1)}[\rho(0)] + \frac{1}{2}\Lambda_t^{(2)}[\rho(0)] =$$

$$= \frac{1 + e^{-ct}}{2}\rho(0) + \frac{1 - e^{-ct}}{4}(\sigma_1\rho(0)\sigma_1 + \sigma_2\rho(0)\sigma_2).$$
(47)

Apparently, Λ_t is a legitimate dynamical map. However, the corresponding generator of evolution has the form:

$$\mathbb{L}_t[\rho(t)] = \sum_{k=1}^3 \gamma_k(t) (\sigma_k \rho(t) \sigma_k - \rho(t)), \tag{48}$$

where the relaxation rates are given by: $\gamma_1 = \gamma_2 = \frac{c}{2}$ and $\gamma_3(t) = -\frac{c}{2} \tanh(c t)$. It is clearly visible now that $\gamma_3(t) < 0$, which means that the operator \mathbb{L}_t (48) generates non-Markovian evolution. Equivalently, we can say that the map Λ_t (47) is not CP-divisible. Therefore, the convex combination of two dynamical maps, each corresponding to a GKSL generator, turns out to generate non-Markovian evolution.

On the other hand, in Ref. [78], the authors introduced a map:

$$\Lambda_t = e^{-\gamma t} \mathbb{I} + (1 - e^{-\gamma t}) \mathcal{E}, \tag{49}$$

where $\mathcal{E}[X] = \sum_{k=1}^{d} |k\rangle \langle k| X |k\rangle \langle k|$ and the set $\{|k\rangle\}_{k=1}^{d}$ constitutes an orthonormal basis in \mathbb{C}^{d} . It was shown that, for a given γ , one is able to find time-dependent $\gamma_{1}(t)$ and $\gamma_{2}(t)$ such that the map Λ_{t} can be represented as [78]:

$$\Lambda_t = p\Lambda_t^{(1)} + (1-p)\Lambda_t^{(2)},$$
(50)

with $\Lambda_t^{(1)} = e^{-\Gamma_k(t)}\mathbb{I} + (1 - e^{-\Gamma_k(t)})\mathcal{E}$ and $\Gamma_k(t) = \int_0^t \gamma_k(\tau) d\tau$. Since neither $\Lambda_t^{(1)}$ nor $\Lambda_t^{(2)}$ is Markovian, one can conclude that the map from (49), which is Markovian and additionally is a semigroup, has been obtained by a convex combination of two non-Markovian semigroups. Mixing two non-Markovian semigroups has made all memory effects disappear and led to a perfectly memoryless evolution.

Apart from the CP-divisibility (Definition 20), there are other methods to demonstrate memory effects in quantum evolution. For example, the non-Markovian behavior of the map Λ_t can be demonstrated by following the criterion given by H.-P. Breuer, E.-M. Lane, and J. Piilo, hereafter referred to as the BLP criterion [72]. However, one must note that the definition of non-Markovianity based on the divisibility property of the dynamical map is not equivalent to the BLP criterion. Examples where these two criteria do not coincide can be found in Ref. [79].

The BLP criterion provides a general measure for the degree of non-Markovianity in open quantum systems. According to the BLP criterion, a dynamical map Λ_t is Markovian if and only if

$$\sigma(t;\rho_1,\rho_2) := \frac{1}{2} \frac{d}{dt} \|\Lambda_t(\rho_1 - \rho_2)\|_{\mathrm{Tr}} \le 0$$
(51)

for all pairs of input states ρ_1 and ρ_2 . The quantity $\sigma(t;\rho_1,\rho_2)$ can be interpreted as the information flow and, as a result, $\sigma(\rho_1,\rho_2;t) < 0$ implies that the information is lost over time (for an isolated system, we have $\sigma(t;\rho_1,\rho_2) = 0$ for all ρ_1,ρ_2 , and $t \ge 0$ since no information is lost due to the absence of interactions with an external environment). On the other hand, $\sigma(t;\rho_1,\rho_2) > 0$ indicates a backflow of information from the environment to the system, which is a proof of non-Markovian effects.

The BLP criterion (51) allows one not only to distinguish a non-Markovian dynamics from a Markovian evolution, but it also leads to a convenient quantifier of the degree of non-Markovianity

$$\mathcal{N} = \max_{\rho_1, \rho_2} \int_{\sigma > 0} \sigma(t; \rho_1, \rho_2) dt,$$
(52)

where the time-integration is performed over all time intervals $(\tau_1^{(k)}, \tau_2^{(k)})$ in which σ is positive, and the maximum is found over all possible pairs of initial states.

Finally, let us comment that the BLP criterion (51) can be explained by the fact that all CPTP maps Λ are contractions for the metric defined through the trace distance. For any two quantum states ρ_1 and ρ_2 , the distance can be defined by $\mathcal{D}(\rho_1, \rho_2) = 1/2 \|\rho_1 - \rho_2\|_{\text{Tr}}$ [26]. Then, the contraction property for any CPTP map Λ can be stated as [80]

$$\mathcal{D}(\Lambda[\rho_1], \Lambda[\rho_2]) \leq \mathcal{D}(\rho_1, \rho_2) \qquad \forall \rho_1, \rho_2 \in \mathcal{S}(\mathcal{H}).$$

For any quantum Markovian process, the trace distance $\mathcal{D}(\Lambda[\rho_1], \Lambda[\rho_2])$, corresponding to any fixed pair of initial states, is a monotonically decreasing function of time. In other words, the distinguishability between any two quantum states declines monotonically, which is interpreted as a flow of information from the system to the environment (consequently, we have $\sigma(t; \rho_1, \rho_2) < 0$). However, for other physical processes, the trace distance does not behave monotonically, which implies that in a certain time interval, the distinguishability of the pair of states increases ($\sigma(t; \rho_1, \rho_2) > 0$). We interpret this phenomenon as a flow of information from the environment back to the system [72].

As has been said, the fundamental problem concerning the conditions that the generator \mathbb{L}_t should satisfy in order to guarantee a legitimate evolution has not been solved yet. Another partially solved problem relates to computing a dynamical map based on a quantum master equation. Both questions remain relevant research problems.

6.3. Nonlocal in Time Approach to Open Quantum Systems Evolution

In an alternative approach to open quantum systems' dynamics one follows the Nakajima–Zwanzig equation, according to which the evolution of a system is given by a nonlocal Equation [81,82]:

$$\frac{d\rho(t)}{dt} = \int_0^t K_{t-\tau}[\rho(\tau)]d\tau,$$
(53)

where K_t denotes an operator called memory kernel. The nonlocal character of evolution given by (53) is associated with the presence of convolution, which mathematically means that the rate of evolution for $\rho(t)$ depends on the history starting from t = 0 (therefore, one needs to integrate the kernel in (53)).

Equation (53) translates into another formula that describes the evolution of a dynamical map:

$$\dot{\Lambda}_t = \int_0^t K_{t-\tau} [\Lambda_\tau] d\tau.$$
(54)

When looking at Equations (53) and (54), one should ask the natural research question. Question: What conditions should the kernel K_t satisfy to guarantee that the map Λ_t obtained from Equation (54) is a legitimate dynamical map?

Unfortunately, there is no concrete answer to this problem. There is only a limited number of specific examples of K_t , for which one can be certain that they provide a legitimate evolution. However, the general construction of the memory kernel remains an unsolved problem.

To analyze the properties of memory kernels, one usually applies the Laplace transform (named after its discoverer Pierre-Simon Laplace). Let us recall its definition.

Definition 24 (Laplace transform). *The Laplace transform of a function* f(t) *is defined for all values* $t \ge 0$ *by the following formula:*

$$\mathcal{L}[f(t)](s) := \int_0^\infty f(t) \, e^{-st} \, dt \equiv \widetilde{f}(s).$$
(55)

Physically speaking, one may say that the function f(t) *is transformed from the time domain into the function* $\tilde{f}(s)$ *in the frequency domain*

By applying the Laplace transform to the evolution equation of the map (54), one obtains a relatively simple relation that connects the Laplace transform of Λ_t and K_t , i.e., Equation (54) transfers into:

$$\widetilde{\Lambda}_s = \frac{1}{s - \widetilde{K}_s},\tag{56}$$

where $\widetilde{\Lambda}_s := \int_0^\infty e^{-st} \Lambda_t dt$ and $\widetilde{K}_s := \int_0^\infty e^{-st} K_t dt$. Equation (56) can be rearranged into a formula for \widetilde{K}_s :

$$\widetilde{K}_s = s \,\mathbb{I} - \widetilde{\Lambda}_s^{-1}. \tag{57}$$

Although there is an explicit formula that connects Λ_s and K_s , it is a very difficult task to determine the conditions that should be satisfied by a legitimate memory kernel. Nevertheless, some specific memory kernels have been found, see, for example, Ref. [83].

7. Conclusions

The paper provides a synthesis of selected topics on open quantum systems. Starting from the fundamental concepts of classical systems, we have gone through quantum semigroups, positive and CP maps, master equations, non-Markovianity, and solvability of TCL equations. The results collected in the paper do not account for the entire theory of open quantum systems but can facilitate entering the field for students and researchers of other expertise.

In the future, we expect further rapid development of the theory of open quantum systems. Then, apart from the advancement of the mathematical formalism, we can observe the emergence of numerous applications in a variety of research areas, including neuronal systems modeling [84], quantum Brownian motion in optomechanical systems [85], or energy transfer processes in photosynthetic complexes [86]. The plethora of mathematical methods and emerging applications make this area a relevant part of modern physics that contributes to the advent of quantum-based technologies.

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Abbreviations

The following abbreviations are used in this manuscript:

BLP	Breuer–Lane–Piilo
СР	completely positive
CPTP	completely positive and trace preserving
GKSL	Gorini-Kossakowski-Sudarshan-Lindblad
NMD	Non-Markovianity degree
TCL	time-convolutionless
UDM	universal dynamical map

References

- 1. Redfield, A.G. On the Theory of Relaxation Processes. *IBM J. Res. Dev.* **1957**, *1*, 19–32.
- 2. Haag, R.; Kastler, D. An Algebraic Approach to Quantum Field Theory. J. Math. Phys. 1964, 5, 848–861. [CrossRef]
- 3. Hellwig, K.-E.; Kraus, K. Pure Operations and Measurements. Commun. Math. Phys. 1969, 11, 214–220. [CrossRef]
- 4. Hellwig, K.-E.; Kraus, K. Pure Operations and Measurements II. Commun. Math. Phys. 1970, 16, 142–147. [CrossRef]
- 5. Kossakowski, A. On quantum statistical mechanics of non-Hamiltonian systems. Rep. Math. Phys. 1972, 3, 247–274. [CrossRef]
- 6. Haake, F. Statistical treatment of open systems by generalized master equations. Springer Tracts Mod. Phys. 1973, 66, 98–168.
- 7. Davis, E.B. *Quantum Theory of Open Systems*; Academic Press: London, UK, 1976.
- Gorini, V.; Kossakowski, A.; Sudarshan, E.C.G. Completely Positive Dynamical Semigroups of N-level Systems. J. Math. Phys. 1976, 17, 821–825. [CrossRef]
- 9. Lindblad, G. On the generators of quantum dynamical semigroups. Commun. Math. Phys. 1976, 48, 119–130. [CrossRef]
- 10. Kraus, K. Operations and effects in the Hilbert space formulation of quantum mechanics. In *Foundations of Quantum Mechanics and Ordered Linear Spaces*; Hartkämper, A., Neumann, H., Eds.; Springer: Berlin/Heidelberg, Germany, 1974; pp. 206–229.
- 11. Kraus, K. States, Effects and Operations, Fundamental Notions of Quantum Theory; Springer: Berlin/Heidelberg, Germany, 1983.
- 12. Bellman, R. Introduction to Matrix Analysis, 2nd ed.; Society for Industrial and Applied Mathematics: Philadelphia, PA, USA, 1997.
- 13. Jacobs, K. Discrete Stochastics. A Series of Advanced Textbooks in Mathematics; Birkhäuser Verlag Basel: Berlin, Germany, 1992; pp. 19–63.
- 14. Ingarden, R.S. Information Theory and Thermodynamics of Light Part II. Principles of Information Thermodynamics. *Fortschr. Phys.* **1965**, *13*, 755–805. [CrossRef]
- 15. Stone, M.H. The Theory of Representations of Boolean Algebras. Trans. Amer. Math. Soc. 1936, 40, 37–111.
- 16. Engel, K.-J.; Nagel, R. One-Parameter Semigroups for Linear Evolution Equations; Springer: New York, NY, USA, 2000.
- 17. Jamiołkowski, A. On Some Aspects of Observability of Stochastic Systems. Open Syst. Inf. Dyn. 2000, 7, 255–276. [CrossRef]
- 18. Kolmogorov, A. Über die analytischen Methoden in der Wahrscheinlichkeitsrechnung. Math. Ann. 1931, 104, 415–458. [CrossRef]

- 19. Norris, J.R. Markov Chains; Cambridge University Press: Cambridge, UK, 1997.
- Thingna, J.; Manzano, D. Degenerated Liouvillians and steady-state reduced density matrices. *Chaos* 2021, 31, 073114. [CrossRef] [PubMed]
- 21. Alicki, R.; Lendi, K. Quantum Dynamical Semigroups and Applications; Springer: Berlin/Heidelberg, Germany, 1987.
- 22. von Neumann, J. Wahrscheinlichkeitstheoretischer Aufbau der Quantenmechanik. Gött. Nach. 1927, 1, 245–272.
- 23. Landau, L. Das Dampfungsproblem in der Wellenmechanik. Z. Phys. 1927, 45, 430–441. [CrossRef]
- 24. James, D.F.V.; Kwiat, P.G.; Munro, W.J.; White, A.G. Measurement of qubits. Phys. Rev. A 2001, 64, 052312. [CrossRef]
- Toninelli, E.; Ndagano, B.; Valles, A.; Sephton, B.; Nape, I.; Ambrosio, A.; Capasso, F.; Padgettm, M.j.; Forbes, A. Concepts in Quantum State Tomography and Classical Implementation with Intense Light: A Tutorial. *Adv. Opt. Photonics* 2019, 11, 67–134. [CrossRef]
- 26. Nielsen, M.A.; Chuang, I.L. Quantum Computation and Quantum Information; Cambridge University Press: Cambridge, UK, 2000.
- 27. Jamiołkowski, A. Fusion Frames and Dynamics of Open Quantum Systems. In *Quantum Optics and Laser Experiments;* Lyagushyn, S., Ed.; InTech: Rijeka, Croatia, 2012; pp. 67–84.
- 28. Yosida, K. Functional Analysis; Springer: Berlin/Heidelberg, Germany, 1995.
- 29. Brezis, H. Functional Analysis, Sobolev Spaces and Partial Differential Equations; Springer: New York, NY, USA, 2011.
- 30. Spohn, H. Kinetic equations from Hamiltonian dynamics: Markovian limits. Rev. Mod. Phys. 1980, 52, 569-615. [CrossRef]
- 31. Stinespring, W.F. Positive functions on C*-algebras. Proc. Amer. Math. Soc. 1955, 6, 211–216.
- 32. Horodecki, M.; Horodecki, P.; Horodecki, R. Separability of Mixed States: Necessary and Sufficient Conditions. *Phys. Lett. A* **1996**, 223, 1–8. [CrossRef]
- 33. Horodecki, R.; Horodecki, P.; Horodecki, M.; Horodecki, K. Quantum entanglement. Rev. Mod. Phys. 2009, 81, 865–942. [CrossRef]
- 34. Benatti, F.; Floreanini, R. Open Quantum Dynamics: Complete Positivity and Entanglement. *Int. J. Mod. Phys. B* 2005, *19*, 3063. [CrossRef]
- 35. Rivas, Á.; Huelga, S.F. Open Quantum Systems. An Introduction; Springer: Berlin/Heidelberg, Germany, 2012.
- Breuer, H.-P.; Laine, E.-M.; Piilo, J.; Vacchini, B. Colloquium: Non-Markovian dynamics in open quantum systems. *Rev. Mod. Phys.* 2016, 88, 021002. [CrossRef]
- 37. Vega, I.; Alonso, D. Dynamics of non-Markovian open quantum systems. Rev. Mod. Phys. 2017, 89, 015001. [CrossRef]
- 38. Mathieu, M. Characterising Completely Positive Elementary Operators. Bull. Lond. Math. Soc. 1998, 30, 603–610. [CrossRef]
- 39. Choi, M.-D. Completely positive linear maps on complex matrices. *Linear Algebra Appl.* **1975**, *10*, 285–290. [CrossRef]
- 40. Chruściński, D. On Time-Local Generators of Quantum Evolution. Open Syst. Inf. Dyn. 2014, 21, 1440004. [CrossRef]
- 41. Jamiołkowski, A. Linear transformations which preserve trace and positive semidefiniteness of operators. *Rep. Math. Phys.* **1972**, *3*, 275–278. [CrossRef]
- 42. Sudarshan, E.C.G.; Mathews, P.M.; Rau, J. Stochastic Dynamics of Quantum-Mechanical Systems. *Phys. Rev.* **1961**, *121*, 920. [CrossRef]
- 43. Salgado, D.; Sanchez-Gomez, J.L.; Ferrero, M. Evolution of any finite open quantum system always admits a Kraus-type representation, although it is not always completely positive. *Phys. Rev. A* **2004**, *70*, 054102. [CrossRef]
- Tong, D.M.; Kwek, L.C.; Oh, C.H.; Chen, J.-L.; Ma, L. Operator-sum representation of time-dependent density operators and its applications. *Phys. Rev. A* 2004, 69, 054102. [CrossRef]
- 45. Breuer, H.-P.; Petruccione, F. The Theory of Open Quantum Systems; Oxford University Press: New York, NY, USA, 2002.
- 46. Blum, K. Density Matrix Theory and Applications, 3rd ed.; Springer: Berlin/Heidelberg, Germany, 2012.
- 47. Schrödinger, E. An Undulatory Theory of the Mechanics of Atoms and Molecules. Phys. Rev. 1926, 28, 1049–1070. [CrossRef]
- 48. Pechukas, P. Reduced Dynamics Need Not Be Completely Positive. *Phys. Rev. Lett.* **1994**, *73*, 1060. [CrossRef]
- 49. Shaji, A.; Sudarshan, E.C.G. Who's afraid of not completely positive maps? Phys. Lett. A 2005, 341, 48–54. [CrossRef]
- 50. Jang, S.; Cao, J.; Silbey, R.J. Fourth-order quantum master equation and its Markovian bath limit. *J. Chem. Phys.* 2002, 116, 2705. [CrossRef]
- Thingna, J.; Zhou, H.; Wang, J.-S. Improved Dyson series expansion for steady-state quantum transport beyond the weak coupling limit: Divergences and resolution. J. Chem. Phys. 2014, 141, 194101. [CrossRef]
- 52. Tanimura, Y.; Kubo, R. Time Evolution of a Quantum System in Contact with a Nearly Gaussian-Markoffian Noise Bath. *Phys. Soc. Jpn.* **1989**, *58*, 101–114. [CrossRef]
- 53. Makri, N.; Makarov, D.E. Tensor propagator for iterative quantum time evolution of reduced density matrices. I. Theory. J. Chem. Phys. 1995, 102, 4600. [CrossRef]
- 54. Alipour, S.; Rezakhani, A.T.; Babu, A.P.; Mølmer, K.; Möttönen, M.; Ala-Nissila, T. Correlation-Picture Approach to Open-Quantum-System Dynamics. *Phys. Rev. X* 2020, *10*, 041024. [CrossRef]
- 55. Chruściński, D.; Pascazio, S. A Brief History of the GKLS Equation. Open Syst. Inf. Dyn. 2017, 24, 1740001. [CrossRef]
- 56. Banks, T.; Susskind, L.; Peskin, M.E. Difficulties for the Evolution of Pure States Into Mixed States. *Nucl. Phys. B* **1984**, 244, 125–134. [CrossRef]
- 57. Manzano, D. A short introduction to the Lindblad master equation. AIP Adv. 2020, 10, 025106. [CrossRef]
- 58. Franke, V.A. On the general form of the dynamical transformation of density matrices. *Theor. Math. Phys.* **1976**, 27, 406–413. [CrossRef]

- 59. Andrianov, A.A.; Ioffe, M.V.; Izotova, E.A.; Novikov, O.O. The Franke-Gorini-Kossakowski-Lindblad–Sudarshan (FGKLS) Equation for Two-Dimensional Systems. *Symmetry* **2022**, *14*, 754. [CrossRef]
- 60. Neudecker, H. A Note on Kronecker Matrix Products and Matrix Equation Systems. *SIAM J. Appl. Math.* **1969**, *17*, 603–606. [CrossRef]
- 61. Hartwig, R.E. AX XB = C, Resultants and Generalized Inverses. SIAM J. Appl. Math. 1975, 28, 154–183. [CrossRef]
- 62. Henderson, H.V.; Searle, S.R. The vec-permutation matrix, the vec operator and Kronecker products: A review. *Linear Multilinear A*. **1981**, *9*, 271–288. [CrossRef]
- Jamiołkowski, A. The minimal Number of Operators for Observability of N-level Quantum Systems. Int. J. Theor. Phys. 1983, 22, 369–376. [CrossRef]
- 64. Czerwinski, A. Optimal evolution models for quantum tomography. J. Phys. A Math. Theor. 2016, 49, 075301. [CrossRef]
- 65. Egger, D.J.; Wilhelm, F.K. Optimal control of a quantum measurement. *Phys. Rev. A* 2014, 90, 052331. [CrossRef]
- 66. Chruściński, D.; Kossakowski, A. Non-Markovian Quantum Dynamics: Local versus Nonlocal. *Phys. Rev. Lett.* **2010**, *104*, 070406. [CrossRef]
- 67. Dyson, F.J. The S matrix in quantum electrodynamics. Phys. Rev. 1949, 75, 1736–1755. [CrossRef]
- 68. Kamizawa, T. On Functionally Commutative Quantum Systems. Open Syst. Inf. Dyn. 2015, 22, 1550020. [CrossRef]
- 69. Czerwinski, A. Open quantum systems integrable by partial commutativity. Phys. Rev. A 2020, 102, 062423. [CrossRef]
- 70. Breuer, H.-P. Genuine quantum trajectories for non-Markovian processes. Phys. Rev. A 2004, 70, 012106. [CrossRef]
- 71. Grigoriu, A.; Rabitz, H.; Turinici, G. Controllability Analysis of Quantum Systems Immersed within an Engineered Environment. *J. Math. Chem.* **2013**, *51*, 1548–1560. [CrossRef]
- 72. Breuer, H.-P.; Laine, E.-M.; Piilo, J. Measure for the Degree of Non-Markovian Behavior of Quantum Processes in Open Systems. *Phys. Rev. Lett.* **2009**, *103*, 210401. [CrossRef] [PubMed]
- 73. Wolf, M.M.; Eisert, J.; Cubitt, T.S.; Cirac, J.I. Assessing Non-Markovian Quantum Dynamics. *Phys. Rev. Lett.* **2008**, 101, 150402. [CrossRef] [PubMed]
- 74. Wolf, M.M.; Cirac, J.I. Dividing Quantum Channels. Commun. Math. Phys. 2008, 279, 147–168. [CrossRef]
- Rivas, Á.; Huelga, S.F.; Plenio, M.B. Entanglement and Non- Markovianity of Quantum Evolutions. *Phys. Rev. Lett.* 2010, 105, 050403. [CrossRef] [PubMed]
- 76. Chruściński, D.; Maniscalco, S. Degree of Non-Markovianity of Quantum Evolution. Phys. Rev. Lett. 2014, 112, 120404. [CrossRef]
- 77. Chruściński, D. Non-Markovianity degree for random unitary evolution. Phys. Rev. A 2015, 91, 012104. [CrossRef]
- 78. Wudarski, F.A.; Chruściński, D. Markovian semigroup from non-Markovian evolutions. Phys. Rev. A 2016, 93, 042120. [CrossRef]
- 79. Chruściński, D.; Kossakowski, A.; Rivas, Á. Measures of non-Markovianity: Divisibility versus backflow of information. *Phys. Rev. A* 2011, *83*, 052128. [CrossRef]
- Ruskai, M.B. Beyond strong subadditivity? Improved bounds on the contraction of generalized relative entropy. *Rev. Math. Phys.* 1994, 6, 1147–1161. [CrossRef]
- 81. Nakajima, S. On Quantum Theory of Transport Phenomena. Prog. Theor. Phys. 1958, 20, 948–959. [CrossRef]
- 82. Zwanzig, R. Ensemble Method in the Theory of Irreversibility. J. Chem. Phys. 1960, 33, 1338–1341. [CrossRef]
- 83. Wudarski, F.A.; Należyty, P.; Sarbicki, G.; Chruściński, D. On admissible memory kernels for random unitary qubit evolution. *Phys. Rev. A* 2015, *91*, 042105. [CrossRef]
- 84. Sun, Y.-J.; Zhang, W.-M. Modeling Neuronal Systems as an Open Quantum System. Symmetry 2021, 13, 1603. [CrossRef]
- 85. Gröblacher, S.; Trubarov, A.; Prigge, N.; Cole, C.D.; Aspelmeyer, M.; Eisert, J. Observation of non-Markovian micromechanical Brownian motion. *Nat. Commun.* **2015**, *6*, 7606. [CrossRef] [PubMed]
- Rebentrost, P.; Aspuru-Guzik, A. Communication: Exciton–phonon information flow in the energy transfer process of photosynthetic complexes. J. Chem. Phys. 2011, 134, 101103. [CrossRef] [PubMed]