Dynamics of open quantum systems initially entangled with environment: Beyond the Kraus representation

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I. INTRODUCTION

Proper understanding of quantum dynamics of open systems is a very important task in many areas of physics ranging from quantum optics to quantum information processing and to quantum cosmology [1]. In general, one can assume an interaction between the open system denoted as A with the environment B. This environment is a quantum system with the Hilbert space of an arbitrary dimension. The whole A plus B system evolves unitarily. In most of the studies on dynamics of open systems it is assumed that the open system and its environment are at the initial moment of their joint evolution factorized [1,2], that is they are described by the density operator of the form

$$\rho_{AB}=\rho_A\otimes\rho_B, \tag{1.1}$$

where ρ_A is the initial state of system A and ρ_B is the initial state of the environment. While the initial state of the open system A may vary the initial state of the environment B is considered to be determined by external conditions. In this context it is natural to ask what is the time evolution of the open system A? Or in other words, what is the explicit form of the map $\$_A:\rho_A\rightarrow\rho_A'$. In order to answer this question one might follow the arguments presented in Ref. [2] and to find the explicit expression for the density operator ρ_A'

$$\begin{aligned}\rho_A'&=\mathrm{Tr}_B(U_{AB}\rho_{AB}U_{AB}^\dagger)\\&=\sum_\mu\langle\mu|U_{AB}\rho_A\otimes\left(\sum_\nu p_\nu|\nu\rangle\langle\nu|\right)U_{AB}^\dagger|\mu\rangle\\&=\sum_{\mu,\nu}\langle\mu|\sqrt{p_\nu}U_{AB}|\nu\rangle\rho_A\langle\nu|\sqrt{p_\nu}U_{AB}^\dagger|\mu\rangle\\&=\sum_{\mu,\nu}M_{\mu\nu}\rho_AM_{\mu\nu}^\dagger,\end{aligned} \tag{1.2}$$

where

$$M_{\mu\nu}=\langle\mu|\sqrt{p_\nu}U_{AB}|\nu\rangle. \tag{1.3}$$

This is the well-known Kraus representation [3] of a superoperator $\$_A$ that has been studied and used in the literature broadly. On the other hand, dynamics of open system in which initial correlations between the system and the environment is taken into account has not been analyzed in detail yet. Taking into account recent interest in quantum entanglement within the context of quantum-information processing it is appropriate to study in detail the role of (quantum) correlations on dynamics of open quantum systems. Some particular aspects of this problem have been discussed in Ref. [4].

In the present paper, we present a general analysis of the role of initial correlations between the open system and an environment on quantum dynamics of the open system.

II. THE ROLE OF INITIAL CORRELATIONS

In this section we will investigate the evolution of an open system A that is initially correlated with the environment B. Let us denote by σ_i the generators of the group SU(N) [5] where N is the dimension of the Hilbert space of the system A. In addition we denote by τ_j the generators of the group SU(M) where M is the dimension of the Hilbert space of the environment B. Using this notation the most general density matrix of the system A and the environment B reads as

$$\rho_{AB}=\frac{1}{NM}(\mathbb{1}_{AB}+\alpha_i\sigma_i\otimes\mathbb{1}_B+\beta_j\mathbb{1}_A\otimes\tau_j+\gamma_{ij}\sigma_i\otimes\tau_j) \tag{2.1}$$

while the density operator of the open system A is obtained via ''tracing'' over the environment

$$\rho_A=\mathrm{Tr}_B(\rho_{AB})=\frac{1}{N}(\mathbb{1}_A+\alpha_i\sigma_i). \tag{2.2}$$

So let us assume that the state (2.1) is the initial state of the whole A plus B system that evolves according to the given unitary matrix U_{AB}. Can we describe in this case the evolution of the subsystem A in the form analogous to Eq. (1.2)? In order to answer the question we have to insert into the equation

$$\rho_A'=\mathrm{Tr}_B(U_{AB}\rho_{AB}U_{AB}^\dagger) \tag{2.3}$$

the expression (2.1) for the density operator ρ_{AB} that results in

$$\rho_A' = \sum_\mu \langle\mu|U_{AB}\frac{1}{N}(\mathbb{1}_A+\alpha_i\sigma_i)\otimes\frac{1}{M}(\mathbb{1}_B+\beta_j\tau_j)U_{AB}^\dagger|\mu\rangle + \sum_\mu \langle\mu|U_{AB}\frac{(\gamma_{ij}-\alpha_i\beta_j)}{NM}\sigma_i\otimes\tau_j U_{AB}^\dagger|\mu\rangle$$

$$= \sum_\mu \langle\mu|U_{AB}(\rho_A\otimes\rho_B)U_{AB}^\dagger|\mu\rangle + \sum_\mu \langle\mu|U_{AB}\frac{(\gamma_{ij}-\alpha_i\beta_j)}{NM}\sigma_i\otimes\tau_j U_{AB}^\dagger|\mu\rangle. \quad (2.4)$$

After rewriting γ_{ij} as $\gamma_{ij}=NM\gamma_{ij}'+\alpha_i\beta_j$ we obtain from Eq. (2.4) the expression

$$\rho_A' = \sum_{\mu,\nu} M_{\mu\nu}\rho_A M_{\mu\nu}^\dagger + \sum_\mu \langle\mu|U_{AB}\gamma_{ij}'\sigma_i\otimes\sigma_j U_{AB}^\dagger|\mu\rangle, \quad (2.5)$$

where the operators $M_{\mu\nu}$ are given by Eq. (1.3). We see that the resulting density operator describing the open system A during the time evolution consists of two terms. The first term corresponds to the standard Kraus representation with no initial correlations as discussed in Sec. I. The second term in the right-hand side of Eq. (2.5) depends *only* on the correlation parameters γ_{ij}' that do not *explicitly* depend on the particular choice of the initial state of the open system A (see below). In other words, these parameters cannot be determined by performing a local measurement on the initial state of the system A.

This second term makes the Eq. (2.5) *inhomogeneous though linear*—we will discuss this consequence of initial correlations between the system and the environment in the following section.

Example 1. We may regard γ_{ij}' as additional parameters that together with the initial state of the environment ρ_B and the unitary operator U_{AB} determine the time evolution of the open system initially prepared in the state ρ_A.

To illustrate the possible significance of γ_{ij}' we will study a simple model describing dynamics of two qubits (spin-1/2 particles). In this model one of the qubits (A) plays the role of the open system while the second qubit (B) plays the role of the environment. Let the unitary evolution operator U_{AB} acting on the joint system of these two qubits is given by the expression

$$U = e^{-iHt} = \mathbb{1}\cos t - iH\sin t, \quad (2.6)$$

where H is the Hamiltonian

$$H = \sigma_x\otimes\frac{1}{2}(\mathbb{1}-\sigma_z)+\mathbb{1}\otimes\frac{1}{2}(\mathbb{1}+\sigma_z), \quad (2.7)$$

with σ_j being Pauli matrices. The interaction described by the Hamiltonian (2.7) corresponds to the well-known controlled-NOT gate [2].

Let us consider two initial conditions $\rho_{AB}^{(1)}$ and $\rho_{AB}^{(2)}$ for the two-qubit state, which in the computer basis $\{|0\rangle,|1\rangle\}$ read

$$\rho_{AB}^{(1)} = |\alpha|^2|00\rangle\langle 00| + |\beta|^2|11\rangle\langle 11|,$$

$$\rho_{AB}^{(2)} = (\alpha|00\rangle+\beta|11\rangle)(\alpha^*\langle 00|+\beta^*\langle 11|). \quad (2.8)$$

Obviously, the qubits A and B in these two-qubit states are in the same state, i.e.,

$$\rho_A^{(1)} = \mathrm{Tr}_B[\rho_{AB}^{(1)}] = \mathrm{Tr}_B[\rho_{AB}^{(2)}] = \rho_A^{(2)},$$

$$\rho_B^{(1)} = \mathrm{Tr}_A[\rho_{AB}^{(1)}] = \mathrm{Tr}_A[\rho_{AB}^{(2)}] = \rho_B^{(2)}. \quad (2.9)$$

On the other hand, the parameters γ_{ij}' in the two-qubit states (2.8) are different. Therefore, this simple model with identical states of subsystems but different correlations will illuminate the role of the correlations on dynamics of open quantum systems.

With the unitary evolution (2.6) the two-qubit systems with the two initial conditions (2.8) evolve at time $t=\pi/2$ into states such that the system A is described by the two density operators

$$\rho_A^{(1)}(t=\pi/2) = \frac{1}{2}(\mathbb{1}+\sigma_3),$$

$$\rho_A^{(2)}(t=\pi/2) = \frac{1}{2}[\mathbb{1}+(|\alpha|^2-|\beta|^2)\sigma_3], \quad (2.10)$$

respectively. We stress here that the open system has been in both cases in the same initial state, i.e., $\rho_A^{(1)}=\rho_A^{(2)} = |\alpha|^2|0\rangle\langle 0|+|\beta|^2|1\rangle\langle 1|$, the environment itself was in both cases, initially, in the same state as well. But due to different initial correlations between the system and the environment the open system has evolved into two different states $\rho_A^{(1)}(\pi/2)$ and $\rho_A^{(2)}(\pi/2)$.

This example illustrates that the initial correlations between the system and its environment may play important role in the dynamics of open systems. Moreover, in most of physical situations such correlations are present and therefore they have to be taken into account.

III. MASTER EQUATION

As follows from our previous discussion, both the state of the environment and the initial correlations between the environment and the open system play significant roles in the dynamics of the open system. Therefore, in order to characterize completely the evolution, it is necessary to determine (fix) the set of the parameters $\{\beta_j\}$, i.e., the state ρ_B of the environment, and the parameters $\{\gamma_{ij}'\}$ describing the correlations. The parameters α_i, β_j, and γ_{ij}' are *arbitrary* conditioned that the matrix ρ_{AB} describe a real physical state of the system AB, that is, it is a density matrix. Specifically, if we represent one particular choice of parameters $\{\alpha_i,\beta_j,\gamma_{ij}'\}$ as a point in a (N^2M^2-1)-dimensional space $\mathbf{R}^{(N^2M^2-1)}$, then the set of physically relevant parameters $\{\alpha_i,\beta_j,\gamma_{ij}'\}$ form a convex subset $\mathcal{S}$ in the space $\mathbf{R}^{(N^2M^2-1)}$. For example, in the case of α_i (the same holds for β_j and γ_{ij}') there is only a subset O_A in the space $\mathbf{R}^{(N^2-1)}$ from which we

can choose the parameters $\{\alpha_i\}$ for which the matrix ρ_{AB} is a physical density matrix. Moreover this subset O_A depends on the choice of the remaining parameters $\{\beta_j\}$ and $\{\gamma'_{ij}\}$. In other words, the subset O_A might be different for different choices of $\{\beta_j\}$ and $\{\gamma'_{ij}\}$. For example, if the system A is initially maximally entangled with the environment then its density operator has to be of the form $\mathbb{1}/N$. On the other hand, if the system A is in a pure state then the only possible initial density matrix of the system A and the environment must have the form $\rho_{AB}=\rho_A\otimes\rho_B$, so that all γ'_{ij} have to be zero. Or, equivalently, if some of the parameters γ'_{ij} are not zero then the state ρ_A cannot be a pure state.

Sometimes it is very useful to describe the evolution of the open system in a form of a master equation. In order to do so we, firstly, rewrite the evolution (2.5) in terms of the left-right superoperator acting on the density operator ρ_A

$$\rho_A(t)=\hat{\mathcal{T}}(t)\rho_A(0)+\xi(t), \tag{3.1}$$

where $\xi(t)$ is the inhomogeneous term that has its origin in the presence of initial correlations between the open system and the environment, i.e., from Eq. (2.5) we have

$$\xi(t)=\sum_{\mu ij}\langle\mu|U_{AB}\gamma'_{ij}\sigma_i\otimes\sigma_j U_{AB}^{\dagger}|\mu\rangle.$$

We stress once again that the operator $\xi(t)$ does not depend *explicitly* on the initial state of the open system A, only the range of possible values of correlations is determined by the choice of ρ_A and ρ_B (see the discussion above). As follows from Eq. (2.5) the left-right action of the superoperator $\hat{\mathcal{T}}(t)$ is equal to the following normal action

$$\hat{\mathcal{T}}(t)\rho_A(0)=\sum_{\mu,\nu}M_{\mu\nu}\rho_A(0)M_{\mu\nu}^{\dagger}.$$

From our previous comments it follows that the choice of the initial correlations restricts a set of density operators ρ_A for which Eq. (3.1) can be used. For instance, for pure states the term $\xi(t)$ is always zero. Therefore, if we would use Eq. (3.1) with nonzero $\xi(t)$ for describing dynamics of an open system initially prepared in a pure state, we might end up with a completely unphysical situation. As discussed above this subset is determined by the condition, that dynamics (1.2) has a physical meaning. This restriction reflects quantum nature of correlations between the system and the environment and have to be taken into account in the derivation of dynamics of open quantum systems that are initially correlated with the environment.

We have to keep in mind that there is always only a subset O_A of all the density matrices of the system A for which the Eq. (3.1) with a given $\xi(t)$ is valid. If, for example, $\xi(t)=0$ then the Eq. (3.1) is valid for all ρ_A and $O_A=\mathcal{S}_A$ where $\mathcal{S}_A$ is a set of all density matrices of the system A. Unless $\xi(t)$ equals to zero O_A is a subset of $\mathcal{S}_A$.

After this preliminary comment we derive the master equation following the formalism presented in Ref. [6]. Differentiating Eq. (3.1) according to time we obtain

$$\frac{\partial}{\partial t}\rho_A(t)=\frac{\partial}{\partial t}\hat{\mathcal{T}}(t)\rho_A(0)+\frac{\partial}{\partial t}\xi(t). \tag{3.2}$$

When we substitute $\rho_A(0)$, which formally can be determined with the help of Eq. (3.1) [7] into Eq. (3.2) we find

$$\frac{\partial}{\partial t}\rho_A(t)=\left(\frac{\partial}{\partial t}\hat{\mathcal{T}}(t)\right)\frac{1}{\hat{\mathcal{T}}(t)}[\rho_A(t)-\xi(t)]+\frac{\partial}{\partial t}\xi(t). \tag{3.3}$$

If we introduce a notation for the Liouvillian superoperator

$$\hat{\mathcal{X}}=\left(\frac{\partial}{\partial t}\hat{\mathcal{T}}(t)\right)\frac{1}{\hat{\mathcal{T}}(t)}, \tag{3.4}$$

then the master equation can be rewritten in the following form

$$\left(\frac{\partial}{\partial t}-\hat{\mathcal{X}}\right)[\rho_A(t)-\xi(t)]=0. \tag{3.5}$$

If the initial correlations were zero, then the master equation (3.5) reduces to the well-known form (see for instance, Ref. [6])

$$\left(\frac{\partial}{\partial t}-\hat{\mathcal{X}}\right)\rho_A(t)=0 \tag{3.6}$$

where the operator $\hat{\mathcal{X}}$ is the same as in Eq. (3.5). Taking into account the fact, that $\xi(t)$ does not depend on the initial state $\rho_A(0)$ we can introduce the operator

$$\mathcal{F}(t)=\left(\frac{\partial}{\partial t}-\hat{\mathcal{X}}\right)\xi(t) \tag{3.7}$$

and rewrite the master equation (3.5) in an inhomogeneous form

$$\left(\frac{\partial}{\partial t}-\hat{\mathcal{X}}\right)\rho_A(t)=\mathcal{F}(t). \tag{3.8}$$

The superoperator $\hat{\mathcal{X}}$ depends only on the initial state of the environment ρ_B and the parameters of the unitary evolution U_{AB}, while the whole information about the initial correlations between the open system and the environment is in the operator $\mathcal{F}(t)$. Finally, we stress once again, that the initial correlations between the open system and the environment determine a class of possible density operators of the open system that can be considered in Eq. (3.8).

IV. DISCUSSION

Till now we have studied how initial correlations between the open system and the environment can influence the time evolution of the open system. We have found that these correlations play an important role that cannot be neglected. In this section we will investigate properties of superoperators (evolutions) $\$_A$ acting on an open system that is a part of the composite system (open system and environment). It is assumed that two parts of the composite system can be initially

correlated. The composite system is considered to be closed so that it evolves unitarily according to a given unitary operator U_{AB}. In what follows we will assume this evolution of the ''Universe'' to be given.

First, we define the most general superoperator (evolution) that originates from a given U_{AB}.

Definition IV.1. Let A is the system of interest, B is the rest of the Universe (the environment), and U_{AB} is a given unitary evolution on the whole system. Let us consider a map

$$\mathcal{P}:\rho_A \rightarrow \rho_{AB}, \tag{4.1}$$

which means that for each ρ_A we choose one ρ_{AB} from a set of all-possible density matrices of the Universe such that

$$\mathrm{Tr}_B(\rho_{AB}) = \rho_A. \tag{4.2}$$

The *superoperator* that describes the most general evolution of the system A is given by the expression

$$\$:\rho_A \rightarrow \rho_A', \tag{4.3}$$

$$\rho_A' \equiv \mathrm{Tr}_B(U_{AB}\rho_{AB}U_{AB}^{\dagger}). \tag{4.4}$$

The map $\mathcal{P}$ in Eq. (4.1) is related to the preparation of the state ρ_A of the system A. We note that while preparing the state ρ_A of the system A the state of the Universe is changed as well. That is, in any act of the preparation of the system A we prepare a state ρ_{AB} rather than an isolated state ρ_A of only the system A without affecting the system B. For this reason ρ_{AB} describes a (correlated) state of the open system and the environment (Universe). Moreover, since the preparation is an act in which a classical information is encoded into a quantum system the map $\mathcal{P}$ is not necessarily linear. Therefore the state $\rho_B = \mathrm{Tr}_A[\rho_{AB}]$ might depend (even in a nonlinear way) on the state ρ_A. For instance we can imagine the map $\mathcal{P}$ of the form $\mathcal{P}(\rho_A) = \rho_A \otimes \rho_A$, which describe the action similar to quantum cloning that obviously is not possible within the framework of linear quantum mechanics, but can easily be performed at the level of preparation of quantum states. Analogously we can imagine a map $\mathcal{P}(\rho_A) = \rho_A \otimes \rho_A^T$, where ρ^T is a transposed state. Taking into account that U_{AB} is fixed then the only ''freedom'' in controlling the dynamics is the choice of the map $\mathcal{P}$.

It is clear from the construction that the superoperator \$ is a trace-preserving map and that the final operator ρ_A' is Hermitian and positive, i.e., it is a valid density matrix. In what follows we will study some aspects of the evolutions of the form IV.1.

(a) From the definition IV.1 it follows that for a given U_{AB} and an arbitrary map $\mathcal{P}$ not all evolutions $\$_A$ can be realized. On the contrary there exists U_{AB} and $\mathcal{P}$ such that a given $\$_A$ can be realized. To see this let us consider a following example.

Example 2. Using the scenario (4.4) we can perform any map $\$:\rho_A \rightarrow \rho_A'$ on a given (known) initial state ρ_A of the system A. Specifically, let $\$:\rho_A \rightarrow \rho_A'$ is a given map. We assume that the map $\mathcal{P}$ acting during the preparation of the system A is such that the composite system has been prepared in the state ρ_{AB}

$$\rho_{AB} = \rho_A \otimes \rho_B,$$

such that $\rho_B = \rho_A'$. The unitary transformation that realizes the desired map is then taken to be

$$U_{AB} = \sum_{i,j} |i\rangle_A\langle j| \otimes |j\rangle_B\langle i|.$$

Obviously, there is nothing surprising here since if we know the initial state of the system ρ_A exactly then we can perform an arbitrary map on the system. In some sense this situation corresponds to a classical physics when a complete knowledge about the state of the system is implicitly always assumed. Knowing the initial state precisely we can perform any map we want [8].

(b) Until now we had not considered the linearity condition in association with the evolution $\$_A$. As we have already commented the unitary evolution U_{AB} is by the definition linear, but the preparation map $\mathcal{P}$ might be nonlinear. At this moment we can ask what conditions on $\mathcal{P}$ have to be imposed so that $\$_A$ is linear. In order to proceed we remind us the definition of the linearity of the evolution $\$_A$. Namely, $\$_A$ is linear if

$$\$_A\left(\sum_j \lambda_j \rho_A^{(j)}\right) = \sum_j \lambda_j \$_A \rho_A^{(j)}. \tag{4.5}$$

Now it is clear that if $\mathcal{P}$ is linear, in a sense that

$$\mathcal{P}\left(\sum_i \lambda_i \rho_A^{(i)}\right) = \sum_i \lambda_i \mathcal{P}(\rho_A^{(i)}) \tag{4.6}$$

then the evolution $\$_A$ is linear. The linearity of $\mathcal{P}$ is a sufficient condition for the linearity of $\$_A$. On the other hand, it is not the necessary condition. We might imagine a nonlinear map $\mathcal{P}$ such that $\$_A$ is linear. To understand this we formally represent the evolution $\$_A$ as $\$_A = \mathrm{Tr}_B U_{AB}$, where we use notation such that $U_{AB}(\rho_{AB}) = U_{AB}\rho_{AB}U_{AB}^{\dagger}$. Then the linearity of $\$_A$ (4.5) can be expressed as

$$\begin{aligned}\mathrm{Tr}_B U_{AB}\mathcal{P}\left(\sum_i \lambda_i \rho_A^{(i)}\right) &= \sum_i \lambda_i \,\mathrm{Tr}_A\, U_{AB}\mathcal{P}(\rho_A^{(i)}) \\ &= \mathrm{Tr}_B\, U_{AB}\left[\sum_i \lambda_i \mathcal{P}(\rho_A^{(i)})\right].\end{aligned} \tag{4.7}$$

From this last equation it follows that if the map $\mathcal{P}$ is linear, then $\$_A$ is linear as well. On the other hand, from the linearity of $\$_A$ does not follow that $\mathcal{P}$ is linear. This is a consequence of the property of the partial trace operation Tr_B. Specifically, from the identity (4.7) the equality

$$U_{AB}\mathcal{P}\left(\sum_i \lambda_i \rho_A^{(i)}\right) = \sum_i \lambda_i U_{AB}\mathcal{P}(\rho_A^{(i)}), \tag{4.8}$$

does not follow.

(c) Next, we will consider consequences of another possible restriction on $\mathcal{P}$. Namely, let us consider a rather fre-

quent condition, that the state of the environment ρ_B does not depend on the state of open system ρ_A. That is

$$\mathrm{Tr}_A \mathcal{P}(\rho_A) = \rho_B = \text{const} \tag{4.9}$$

for all ρ_A. If ρ_A is pure, then under the condition (4.9) the map $\mathcal{P}$ is uniquely defined such that $\mathcal{P}(\rho_A) = \rho_A \otimes \rho_B$. On the other hand, if ρ_A is impure, then under the condition (4.9) the map $\mathcal{P}$ might not be uniquely specified, i.e., correlation between A and B can play a role.

If the condition (4.9) is fulfilled and in *addition* the evolution $\$_A$ in the definition IV.1 is linear, then the map $\mathcal{P}$ can be chosen such that $\mathcal{P}(\rho_A) = \rho_A \otimes \rho_B$ for all ρ_A. But this means that the evolution $\$_A$ can be represented in the Kraus representation [3]. Consequently, this map is completely positive [2].

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[5] To be mathematically correct σ_i are not generators of the corresponding group but σ_i multiplied by the complex constant i. The complex constant is usually omitted and the σ_i alone are called generators. The same remark holds for generators τ_j.

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[7] This inversion is possible due to the fact that in the *finite-dimensional* Hilbert spaces matrix elements of density operators are analytic functions. Consequently, $\hat{\mathcal{T}}(t)$ are nonsingular operators (except maybe for a set of *isolated* values of t) in which case the inverse operators $\hat{\mathcal{T}}(t)^{-1}$ do exist.

[8] Here we emphasize that we *can* choose the factorized density operator. It does not mean that the correlated density operator cannot be used. For more discussion see the end of the previous paragraph.