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

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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.

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. 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 \(A + B\) 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, that is they are described by the density operator of the form

\[
\rho_{AB} = \rho_A \otimes \rho_B
\]  

(1.1)

where \(\rho_A\) is the initial state of system \(A\) and \(\rho_B\) 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 \(S_A : \rho_A \rightarrow \rho_A'\)? 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 \(\rho_A'\):

\[
\rho_A' = \text{Tr}_B (U_{AB} \rho_{AB} U_{AB}^\dagger)
\]

\[
= \sum_{\mu} \langle \mu | U_{AB} \rho_A \otimes \left( \sum_{\nu} p_{\nu} |\nu\rangle \langle \nu| \right) U_{AB}^\dagger |\mu\rangle
\]

\[
= \sum_{\mu,\nu} \langle \mu | \sqrt{p_{\nu}} U_{AB} |\nu\rangle \rho_B |\nu\rangle \sqrt{p_{\nu}} U_{AB}^\dagger |\mu\rangle
\]

\[
= \sum_{\mu,\nu} M_{\mu\nu} \rho_B M_{\mu\nu}^\dagger,
\]  

(1.2)

where

\[
M_{\mu\nu} = \langle \mu | \sqrt{p_{\nu}} U_{AB} |\nu\rangle.
\]  

(1.3)

This is the well known Kraus representation of a super-operator \(S_A\) which 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 earlier in Refs. \([4,5]\). In particular, in Ref. \([4]\) decoherence and initial correlations in quantum Brownian motion have been analyzed, while in Refs. \([5,6]\) a motion of a free particle coupled to a linearly dissipative environment has been studied. The connection between the initial correlations and the complete positivity has been discussed in Ref. \([5]\).

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 \(A\) which is initially correlated with the environment \(B\). Let us denote by \(\sigma_i\) the generators of the group \(SU(N)\) where \(N\) is the dimension of the Hilbert space of the system \(A\). In addition we denote by \(\tau_j\) 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

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

(2.1)

while the density operator of the open system \(A\) is obtained via “tracing” over the environment

\[
\rho_A = \text{Tr}_B (\rho_{AB}) = \frac{1}{N} (\mathbb{1}_A + \alpha_i \sigma_i).
\]

(2.2)

So let us assume that the state \((2.1)\) is the initial state of the whole \(A + B\) system which 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. (1.3)? In order to answer the question we have to insert into the equation

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

the expression (2.1) for the density operator $\rho_{AB}$ which results in

$$
\rho_A' = \sum_\mu \langle \mu | U_{AB} \frac{1}{N} (1_A + \alpha_\mu \sigma_\mu) \otimes \frac{1}{N'} (1_B + \beta_\mu \tau_\mu) U_{AB}^\dagger | \mu \rangle

+ \sum_\mu \langle \mu | U_{AB} \frac{\gamma_\mu - \alpha_\mu \beta_\mu}{NM} \sigma_\mu \otimes \tau_\mu 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_\mu - \alpha_\mu \beta_\mu}{NM} \sigma_\mu \otimes \tau_\mu U_{AB}^\dagger | \mu \rangle \tag{2.4}
$$

After rewriting $\gamma_\mu$ as $\gamma_\mu = NM \gamma_\mu' + \alpha_\mu \beta_\mu$ we obtain from Eq. (2.4) the expression

$$
\rho_A' = \sum_{\mu,\nu} M_{\mu\nu} \rho_A M_{\nu\mu}^\dagger

+ \sum_\mu \langle \mu | U_{AB} \gamma_\mu' \sigma_\mu \otimes \sigma_\mu U_{AB}^\dagger | \mu \rangle, \tag{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. II. The second term in the right-hand side of Eq. (2.5) depends only on the correlation parameters $\gamma_\mu'$ which 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 equation (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 $\gamma_\mu'$ as additional parameters which together with the initial state of the environment $\rho_B$ and the unitary operator $U_{AB}$ determine the time evolution of the open system initially prepared in the state $\rho_A$.

To illustrate the possible significance of $\gamma_\mu'$ 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

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

where $H$ is the Hamiltonian

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

with $\sigma_z$ being Pauli matrices. The interaction described by the Hamiltonian (2.7) corresponds to the well-known controlled-NOT gate $\text{CNOT}$.

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

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

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

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

$$
\rho_A^{(1)} = \text{Tr}_B \rho_A^{(1)} = \text{Tr}_B \rho_A^{(2)} = \rho_A^{(2)},

\rho_B^{(1)} = \text{Tr}_A \rho_A^{(1)} = \text{Tr}_A \rho_A^{(2)} = \rho_B^{(2)}. \tag{2.9}
$$

On the other hand the parameters $\gamma_\mu'$ 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], \tag{2.10}
$$

respectively. We stress here that the open system has been in both cases in the same initial state, i.e. $\rho_A^{(1)} = \rho_A^{(2)} = |\alpha|^2 |00\rangle \langle 00| + |\beta|^2 |11\rangle \langle 11|$, 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 role 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 \( \rho_B \) of the environment, and the parameters \( \{ \gamma_{ij}' \} \) describing the correlations. The parameters \( \alpha_i, \beta_j \) and \( \gamma_{ij}' \) are arbitrary conditioned that the matrix \( \rho_{AB} \) 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 \( (N^2, M^2 - 1) \) dimensional space \( \mathbb{R}^{(N^2, M^2 - 1)} \), then the set of physically relevant parameters \( \{ \alpha_i, \beta_j, \gamma_{ij}' \} \) form a convex subset \( S \) in the space \( \mathbb{R}^{(N^2, M^2 - 1)} \). For example, in the case of \( \alpha_i \) (the same holds for \( \beta_j \) and \( \gamma_{ij}' \)) there is only a subset \( O_A \) in the space \( \mathbb{R}^{(N^2-1)} \) from which we can chose the parameters \( \{ \alpha_i \} \) so that the density matrix \( \rho_{AB} \) is a reasonable 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 \( O_A \) is different for different choices of \( \{ \beta_j \} \) and \( \{ \gamma_{ij}' \} \). For example, 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 \( \gamma_{ij}' \) have to be zero. Or equivalently if some of the parameters \( \gamma_{ij}' \) are not zero then the state \( \rho_{AB} \) can’t be a pure state.

Sometimes it’s 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 (2.3) in terms of the left-right super-operator acting on the density operator \( \rho_A \)

\[
\rho_A(t) = \hat{T}(t) \rho_A(0) + \xi(t),
\]

where \( \xi(t) \) is the inhomogeneous term which has its origin in the presence of initial correlations between the open system and the environment, i.e. from Eq. (2.3) 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 \( \rho_A \) and \( \rho_B \) (see the discussion above). As follows from Eq. (2.5) the left-right action of the super-operator \( \hat{T}(t) \) is equal to the following normal action

\[
\hat{T}(t) \rho_A(0) = \sum_{\mu \nu} M_{\mu \nu} \rho_A(0) M_{\nu \mu}^\dagger.
\]

From our previous comments it follows that the choice of the initial correlations restricts a set of density operators \( \rho_A \) 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 (3.2) 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 which are initially correlated with the environment.

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

After this preliminary comments we derive the master equation following the formalism presented in Ref. [8]. Differentiating Eq. (3.1) according to time we obtain

\[
\frac{\partial}{\partial t} \rho_A(t) = \frac{\partial}{\partial t} \hat{T}(t) \rho_A(0) + \frac{\partial}{\partial t} \xi(t)
\]

When we substitute \( \rho_A(0) \) which formally can be determined with the help of Eq. (3.4) into (3.2) we find

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

If we introduce a notation for the Liouvillian superoperator

\[
\hat{X} = \left( \frac{\partial}{\partial t} \hat{T}(t) \right) \frac{1}{T(t)}
\]

then the master equation can be rewritten in the following form

\[
\left( \frac{\partial}{\partial t} - \hat{X} \right) [\rho_A(t) - \xi(t)] = 0
\]

If the initial correlations were zero, then the master equation (3.2) reduces to the well known form (see for instance, Ref. [8])

\[
\left( \frac{\partial}{\partial t} - \hat{X} \right) \rho_A(t) = 0
\]

where the operator \( \hat{X} \) is the same as in Eq. (3.2). Taking into account the fact, that \( \xi(t) \) does not depend on the initial state \( \rho_A(0) \) we can introduce the operator

\[
\mathcal{F}(t) = \left( \frac{\partial}{\partial t} - \hat{X} \right) \xi(t)
\]

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

\[
\left( \frac{\partial}{\partial t} - \hat{X} \right) \rho_A(t) = \mathcal{F}(t).
\]

We stress once again that the super-operator \( \hat{X} \) depends only on the initial state of the environment \( \rho_B \) 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 \( \mathcal{F}(t) \).
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 which cannot be neglected. In this section we will investigate properties of super-operators (evolutions) $\mathcal{S}_A$ acting on an open system which is a part of the composite system (open system + 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.

Firstly we define the most general super-operator (evolution) which 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

$$\mathcal{P} : \rho_A \rightarrow \rho_{AB}$$

which means that for each $\rho_A$ we choose one $\rho_{AB}$ from a set of all possible density matrices of the Universe such that

$$\text{Tr}_B(\rho_{AB}) = \rho_A$$

The super-operator which describes the most general evolution of the system $A$ is given by the expression

$$\mathcal{S} : \rho_A \rightarrow \rho_A'$$

$$\rho_A' \equiv \text{Tr}_B \left( U_{AB} \rho_{AB} U_{AB}^\dagger \right)$$

The map $\mathcal{P}$ in Eq. (11) is related to the preparation of the state $\rho_A$ of the system $A$. We note that while preparing the state $\rho_A$ 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 $\rho_{AB}$ rather than an isolated state $\rho_A$ of only the system $A$ without affecting the system $B$. For this reason $\mathcal{P}$ 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 $\rho_B = \text{Tr}_A[\rho_{AB}]$ might depend (even in a nonlinear way) on the state $\rho_A$. 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 which 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 $\rho_A^T$ 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 super-operator $\mathcal{S}$ is a trace preserving map and that the final operator $\rho_A'$ is Hermitian and positive, i.e., it is a valid density matrix. In what follows we will study some aspects of the 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 $\mathcal{S}_A$ can be realized. On the contrary there exists $U_{AB}$ and $\mathcal{P}$ such that a given $\mathcal{S}_A$ can be realized. To see this let us consider a following example.

**Example 2.** Using the scenario (4.4) we can perform any map $\mathcal{S} : \rho_A \rightarrow \rho_A'$ on a given (known) initial state $\rho_A$ of the system $A$. Specifically, let $\mathcal{S} : \rho_A \rightarrow \rho_A'$ 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 $\rho_{AB}$

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

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

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

Obviously, there is nothing surprising here since if we know the initial state of the system $\rho_A$ 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.

b. Till now we had not considered the linearity condition in association with the evolution $\mathcal{S}_A$. 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 which conditions on $\mathcal{P}$ to has to be imposed so that $\mathcal{S}_A$ is linear. In order to proceed we remind us the definition of the linearity of the evolution $\mathcal{S}_A$. Namely, $\mathcal{S}_A$ is linear if

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

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

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

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

\[
\text{Tr}_B U_{AB} \mathcal{P} \left( \sum_i \lambda_i \rho_A^{(i)} \right) = \sum_i \lambda_i \text{Tr}_A U_{AB} \mathcal{P}(\rho_A^{(i)}) \tag{4.7}
\]

\[ = \text{Tr}_B U_{AB} \left[ \sum_i \lambda_i \mathcal{P}(\rho_A^{(i)}) \right] \]

From this last equation it follows that if the map \( \mathcal{P} \) is linear, then \( \mathcal{S}_A \) is linear as well. On the other hand from the linearity of \( \mathcal{S}_A \) does not follow that \( \mathcal{P} \) is linear. This is a consequence of the property of the partial trace operation \( \text{Tr}_B \). Specifically, from the identity \( 4.3 \) 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 frequent condition, that the state of the environment \( \rho_B \) does not depend on the state of open system \( \rho_A \). That is

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

for all \( \rho_A \). If \( \rho_A \) is pure, then under the condition \( 4.3 \) the map \( \mathcal{P} \) is uniquely defined such that \( \mathcal{P}(\rho_A) = \rho_A \otimes \rho_B \). On the other hand if \( \rho_A \) 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 \( \mathcal{S}_A \) 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 \( \rho_A \). But this means that the evolution \( \mathcal{S}_A \) can be represented in the Kraus representation \( 4.4 \). Consequently, this map is completely positive \( 2 \).

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