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NON-MARKOVIAN OPEN QUANTUM SYSTEMS: SYSTEM–ENVIRONMENT CORRELATIONS IN DYNAMICAL MAPS

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We construct a non-Markovian dynamical map that accounts for systems correlated to the environment. We refer to it as a canonical dynamical map, which forms an evolution family. The relationship between inverse maps and correlations with the environment is established. The mathematical properties of complete positivity is related to classical correlations, according to quantum discord, between the system and the environment. A generalized non-Markovian master equation is derived from the canonical dynamical map.

Keywords: Open systems; positive maps.

1. Introduction

The theory of dynamical maps for open quantum systems was first introduced as the quantum generalization of classical stochastic processes.[1] The evolution of a system that interacts with an environment, is fully given by a dynamical map that corresponds to a quantum stochastic process. The state, the environment, and the correlations between them, change with time. To obtain the Kossakowski−Lindblad master equation,[2−5] microscopic models where the environment is refreshed is needed. By refreshing the environment, it does not evolve in time such that it behaves like an ideal bath. This refreshing effectively discards the gained correlations, such that they are now inaccessible and can never decrease.

In this paper we study the significance of such correlations. In particular, we show how they are the effective memory Kernel of non-Markovian dynamics. We also connect the classical correlations, as measured by quantum discord[6,7] to completely positive non-Markovian maps. This provides a unified view between bipartite correlations and memory effects in non-Markovian dynamics.

A dynamical map of a system that was uncorrelated from the environment at t_0 might develop correlations through time. These correlations change the map such that at time t_1,

$$\mathbb{B}_{(t_2|t_0)} \neq \mathbb{B}_{(t_2|t_1)} \star \mathbb{B}_{(t_1|t_0)}. \tag{1}$$

When the Markov approximation is assumed to be valid, the map then takes the form:

$$\mathbb{B}_{(t_2|t_0)} \approx \mathbb{B}_{(t_2|t_1)} \star \mathbb{B}_{(t_1|t_0)}, \tag{2}$$

with $t_{i+1} - t_i = \Delta t$ for all i. The maps now form a dynamical semigroup that depends on the parameter Δt. This approximation was used by Kossakowski to derive a family of equations of motion for open quantum system[2–4] that lead to irreversible behavior, where the master equation can be interpreted as the time derivative of the completely positive dynamical maps.

Altogether, discarding the system−environment correlations do allow a description of dissipation, but it has important limitations.[8–19] First, the Markov approximation can lead to unphysical results.[20] States with initial environmental correlations can have not completely positive dynamics.[21] The discarded higher orders of t introduce irreversibility into the equation.[22] Finally, the semigroup property has an essential exponential decay rate for short times. As illustrated by the quantum Zeno effect,[23] this is not permitted. All these highlight the limitations introduced by ignoring the role of system−environment correlations.

Extensions to the theory of open quantum systems that can go beyond the Markov approximation have been developed,[24,25] but the importance of the system−environment correlations in them has been ignored. In this paper, we develop a generalization of dynamical maps for open quantum systems to states correlated with their environment, and we show how these correlations are responsible for non-Markovian dynamics. Non-Markovian dynamics are such that to consistently evolve a system, additional information beyond just the system's state, is needed. This additional information is referred to as memory.

This paper is organized as follows. First, we review the theory of stochastic processes for quantum systems in Sec. 2. Different forms of the dynamical maps, their inverses, and mathematical properties are discussed. In Sec. 3, we study how initial correlations between the system and the environment are the crucial element of non-Markovian dynamics. We then construct what we call a *canonical dynamical map*, as first introduced in Refs. 26 and 27, that is fully non-Markovian.[a] We show how the constrain imposed by the correlations act as the memory kernel. We discuss how the quantum nature of the correlations, as defined by quantum discord,

[a] The term canonical is used to remind us that this map effectively contains all the system−environment dynamics without any approximation.

determine the mathematical properties of the non-Markovian map. We then propose a canonical embedding map that dynamically determines how the system is correlated to the environment at all times. In Sec. 4, we derive the generalized non-Markovian master equation. The equation is local in time if we allow for system–environment correlations. We then show how to introduce irreversibility by discarding terms of higher order in time. This truncation does not eliminate all the system–environment correlations, and leads to dissipation beyond the Markovian regime. We discuss the connection of the non-Markovian master equation to previous instances of specific non-Markovian master equations and make the concluding remarks in Sec. 6. The theory of non-Markovian dynamical maps developed here provides a way to describe decoherence phenomena beyond the Kossakowski–Lindblad master equation from the understanding of the dynamical role of system–environment correlations.

2. Quantum Stochastic Processes and Definitions

We start the paper by reviewing the important concepts and definitions of quantum stochastic processes. We use density matrix η to describe the most general quantum mechanical state of a system. The density matrix must have unit trace, Hermiticity, and non-negative eigenvalues.[28] If we write the density matrices using tensor notation, a quantum stochastic process acts just like a classical stochastic process. A quantum stochastic supermatrix $\mathbb{B}$ can be defined to describe the most general evolution of an initial density matrix $\eta(i)$ to a final density matrix $\eta(f)$, such that $\eta(i)_{rs} \to \eta(f)_{r's'} = \mathbb{B}_{r'r,s's}\eta(i)_{rs}$ in tensor notation, where repeated indices are summed. The quantum stochastic supermatrix has properties that guarantees the preservation of the trace of the density matrix, as well as its Hermiticity. If a map transforms all non-negative matrices into non-negative matrices, it is said to have the property of *positivity.*[1] In Sec. 3.2, we study physical situations where the positivity condition must be reinterpreted from the significance of system–environment correlations. For now, we decompose $\mathbb{B}$ into its eigenmatrices $\{\mathrm{C}_\alpha\}$ and real eigenvalues $\{\lambda_\alpha\}$. The action of the map is then:

$$\eta(f) \equiv \sum_\alpha \lambda_\alpha \mathrm{C}_\alpha \eta(i) \mathrm{C}_\alpha^\dagger. \tag{3}$$

Note that $\{\mathrm{C}_\alpha\}$ are linearly independent and trace orthogonal, $\mathrm{Tr}[\mathrm{C}_\alpha^\dagger \mathrm{C}_\beta] = 0$ for $\alpha \neq \beta$. Hermiticity of η is automatically preserved by the multiplication on the left and right. The trace of η is preserved by the condition $\sum_\alpha \lambda_\alpha \mathrm{C}_\alpha^\dagger \mathrm{C}_\alpha = \mathbb{I}$. Preserving the non-negative eigenvalues of the density matrix is implicit. A stronger condition than positivity, *complete positivity*, is very natural now. Complete positivity is defined as having all non-negative eigenvalues $\lambda_\alpha \geq 0$.[29,30] While positivity is a condition on the action of the map on density matrices, complete positivity is a condition on the map itself. Much attention has been given to this class of maps, but confining quantum evolution to them has proven to be too restrictive.[9,31–36]

2.1. *Dynamical maps of open quantum systems*

The evolution of a closed quantum system is generated by a unitary operator $U_{(t_f|t_i)}$ and can also be viewed as a stochastic process through a unitary map, $\mathbb{U}_{(t_f|t_i)}\rho(t_i) \equiv U_{(t_f|t_i)}\rho(t_i)U^\dagger_{(t_f|t_i)} = \rho(t_f)$. This map is completely positive.

However, we are interested in the evolution of an open quantum system. In this case, the total state $\rho^{\mathcal{SE}}$ has a part that is accessible to us, the system $\mathcal{S}$, and one that is inaccessible, a finite-dimensional environment $\mathcal{E}$. The reduced density matrix of the system is found by tracing out the environmental variables, $\eta^{\mathcal{S}} = \mathrm{Tr}_{\mathcal{E}}[\rho^{\mathcal{SE}}]$.[b] If we only monitor the evolution of the system, it is generally nonunitary and best described by a dynamical map of the form:

$$\mathbb{B}_{(t_f|t_i)}\eta(t_i) \equiv \mathrm{Tr}_{\mathcal{E}}[U_{(t_f|t_i)}\rho(t_i)U^\dagger_{(t_f|t_i)}] = \eta(t_f). \tag{4}$$

In the total space, the evolution is given by the unitary map $\mathbb{U}$, while in the reduced space we get a more complicated evolution. This is represented by the following diagram:

$$\begin{array}{ccl} \rho(t_i) & \leftrightarrow & \rho(t_f) = U_{(t_f|t_i)}\rho(t_i)U^\dagger_{(t_f|t_i)} \\ \downarrow & & \downarrow \\ \eta(t_i) & \rightarrow & \eta(t_f) = \mathrm{Tr}_{\mathcal{E}}[\rho(t_f)]. \end{array} \tag{5}$$

The top level of the diagram represents the unitary evolution of the total system. The lower level is the reduced system and its open evolution. To go from the total space to the reduce space, or "down" as indicated by the arrows, we use the trace map $\mathbb{T}$, that acts in the following manner: $\mathbb{T}\rho^{\mathcal{SE}} \equiv \mathrm{Tr}_{\mathcal{E}}\rho^{\mathcal{SE}} = \eta$. Note that there is no arrow to go from $\eta \to \rho$, or "up." In general, there is no map that inverts the trace such that $\tilde{\mathbb{T}} \star \mathbb{T}\rho^{\mathcal{SE}} = \rho^{\mathcal{SE}}$. But, for now, let's assume that we can construct a map that, with some additional information, can invert the trace. We will refer to it as the embedding map $\mathbb{E}$. With such a map, the dynamical map for the process from $\eta(t_i) \to \eta(t_f)$ can be expressed as the composition of three maps,

$$\mathbb{B}_{(t_f|t_i)} \equiv \mathbb{T} \star \mathbb{U}_{(t_f|t_i)} \star \mathbb{E}. \tag{6}$$

First, the trace is inverted to go from the reduced to the total space, then a unitary map evolves the total state and finally a trace reduces it to the system part of the space. When $t_f = t_i$, there is no evolution and the map is just unity.

The difficulty of inverting the trace comes from the system−environment correlations. Any inverse would need enough information to reestablish these correlations. In other words, inverting the trace would depend on a kernel that comes from correlations of the system with the environmental variables. In Sec. 3.4, we will derive a pseudoinverse, an embedding map $\mathbb{E}$, that inverts the trace based on the physical considerations of the dynamics of the total state. This embedding will

[b] The total system−environment space will be denoted by ρ, while the reduced system state by η. Superscripts to indicate the system $\mathcal{S}$ and environment $\mathcal{E}$ will be suppressed when their meaning is clearly implied.

assume additional information about the system–environment correlations. For now, to illustrate the rule of embeddings, we study the simpler case where there are no correlations between the system and the environment.

2.2. *Initially uncorrelated states*

A standard assumption in open systems of the form Eq. (4) is that the system and environment are, at the initial time, in a tensor (Kronecker) product of two density matrices, $\rho^{\mathcal{SE}}(t_i) = \eta^{\mathcal{S}}(t_i) \otimes \tau^{\mathcal{E}}$. This is equivalent to assuming that there are no correlations between the system and the environment. For an analysis of how this assumption is disconnected from realistic experimental limitations, see Refs. 8–10,21 and 37. This very restrictive assumption can be shown to lead to dynamical maps that, in the form of Eq. (3), have non-negative eigenvalues.[10] This is proved by breaking the corresponding dynamical map into the composition of several completely positive maps,[9] as in Eq. (6). The trace $\mathbb{T}$ and the unitary map $\mathbb{U}$ are both completely positive. An embedding map $\mathbb{E}$ can be defined to that take the system state at the initial time, and embed it into the system–environment space[9,31,38]:

$$\mathbb{E}_{t_i}(\eta(t_i)) = \eta(t_i) \otimes \tau. \tag{7}$$

Since τ has positive eigenvalues, the embedding map can be written as $\mathbb{E}(\eta) = (\mathbb{I}^{\mathcal{S}} \otimes \sqrt{\tau^{\mathcal{E}}})\eta^{\mathcal{S}}(\mathbb{I}^{\mathcal{S}} \otimes \sqrt{\tau^{\mathcal{E}}})^\dagger$, which is of the form of Eq. (3) with non-negative eigenvalues. The dynamical map that takes a state without initial correlations with its environment is the composition of three completely positive maps: embedding, unitary evolution, and reduction. Initially uncorrelated states are not the only states that can give rise to completely positive maps.[9,35]

The embedding map presented here is only applicable to the system at time t_i. At other times it might have developed correlations with the environment and not be of the product form. A generalization of this map for all times will be presented in Sec. 3.4.

3. Non-Markovian Dynamical Maps

The Markov approximation relies on discarding correlations between the system and its environment, and is incompatible with a general theory of open quantum systems. In the previous section, we discussed how this approximation was taken to obtain an approximated composition property from Eq. (2) that permits the definition of the derivative of the map. By relaxing these assumptions, we can allow for not completely positive dynamical maps and thus account for physically meaningful correlations with the environment. We obtain the composition property by accounting for these correlations. First, we illustrate how even when a system is uncorrelated from its environment, correlations developed at other times act as memory effects in the non-Markovian dynamics.

3.1. *Initially correlated states*

We will show how correlations between the system and its environment are developed, and their role in open system dynamics. We will study the case where the tensor product of a system and environment state at time t_0 can be evolved to develop correlations. Their dynamical map to time t_2 is computed as before,

$$\begin{array}{ccc} \rho(t_0) = \eta(t_0) \otimes \tau & \leftrightarrow & \rho(t_2) = \mathbb{U}_{(t_2|t_0)}(\rho(t_0)) \\ \downarrow & & \downarrow \\ \eta(t_0) & \rightarrow & \mathbb{B}_{(t_2|t_0)}(\eta(t_0)) = \eta(t_2). \end{array} \tag{8}$$

To define the map $\mathbb{B}_{(t_2|t_0)}$ we need the composition of three maps. First, one that inverts the trace at t_0, to have an arrow that goes from $\eta(t_0) \rightarrow \rho(t_0)$. This can be accomplished by the embedding map from Eq. (7). Then we have a unitary map $\mathbb{U}_{(t_2|t_0)}$. At time t_2 we have a trace to go from $\rho(t_0) \rightarrow \eta(t_0)$. To obtain Eq. (6) from Eq. (8), we go from $\eta(t_0) \rightarrow \eta(t_2)$ by starting on the bottom-left of the diagram, go up, then to the right, and then down.

If we introduce an intermediate time t_1, the evolution becomes,

$$\begin{array}{ccccc} \rho(t_0) & \leftrightarrow & \rho(t_1) = \mathbb{U}_{(t_1|t_0)}(\rho(t_0)) & \leftrightarrow & \rho(t_2) = \mathbb{U}_{(t_2|t_1)}(\rho(t_1)) \\ \downarrow & & \downarrow & & \downarrow \\ \eta(t_0) & \rightarrow & \mathbb{B}_{(t_1|t_0)}(\eta(t_0)) = \eta(t_1) & \rightarrow & \mathbb{B}_{(t_2|t_1)}(\eta(t_1)) = \eta(t_2). \end{array} \tag{9}$$

Here, $\mathbb{B}_{(t_2|t_0)}$ as well as $\mathbb{B}_{(t_1|t_0)}$ are completely positive, but $\mathbb{B}_{(t_2|t_1)}$ might come from a $\rho(t_1) \neq \eta(t_1) \otimes \tau$. Not completely positive maps $\mathbb{B}_{(t_2|t_1)}$ can come from system−environmental correlations at t_1, such as entanglement[31] and more generalized quantum correlations,[9,35] such as the ones defined by quantum discord.[6,39]

To develop a prescription to consistently describe maps for initially correlated states, we need to find an effective inverse of the trace at time t_1, $\mathbb{T}\rho(t_1) = \eta(t_1)$, an embedding $\mathbb{E}_{t_1}$ such that $\eta(t_1) \rightarrow \rho(t_1)$, use the inverse to find dynamical map. Inverting the trace was accomplished in Sec. 2.2 by introducing a completely positive embedding map, Eq. (7). For initially correlated states it is necessary to relax the positivity condition. We study how these not completely positive maps inverse maps have a physical interpretation if we account for non-Markovian quantum dynamics.

3.2. *Correlations and inverse dynamical maps*

We will now discuss the connection between the role of initial system−environment correlations to the problem of inverting the dynamics of an open system. We will show how the difficulties of establishing an embedding map that accounts for system−environment correlations is the same problem as that of inverting the dynamics of $\mathbb{B}$ by a pseudoinverse dynamical map $\tilde{\mathbb{B}}$. The matrix for the map $\tilde{\mathbb{B}}$ is positive only on a convex domain consisting of a subset of all density matrices that correspond to the image for $\mathbb{B}$. In other words, its action is only well behaved on the subset $\{\eta'\}$ of density matrices of the form $\eta' = \mathbb{B}\,\eta$ for all $\{\eta\}$. This subset is called the *compatibility domain*.[c] Inverse maps are generally not completely positive.[41] We will show how the complete positivity condition is incompatible with non-Markovian open quantum systems due to the role of system−environment correlations and the nonpositivity of inverse maps.

The correlations at t_1, by definition, limit the valid domain of states at that time. Identically, the history from $[t_0, t_1]$ can limit the domain at time t_1. We propose to interpret these correlations as a consequence of the memory effects from $[t_0, t_1]$. Non-Markovian dynamics are obtained from system variables that are correlated with outside variables.

A consistent way to define maps after they have developed correlations is with inverse dynamical maps. To define the inverse dynamical map, additional information is necessary. This additional information is the history from the unitary evolution. From this, the inverse dynamical map $\tilde{\mathbb{B}}_{(t_i|t_f)}$ can be found, which is generally not a positive map. $\tilde{\mathbb{B}}_{(t_i|t_f)}$ can only be meaningfully applied to the set $\mathbb{B}_{(t_f|t_i)}\eta(t_i)$ for all density matrices $\{\eta(t_i)\}$. The compatibility domain is identical to the set of states compatible with the history from $[t_0, t_1]$. States outside the compatibility domain will be inconsistent with its history, and when its evolution is reversed it may not be mapped to a valid physical state. There is no reason for these maps to be positive, much less completely positive. On the contrary, history effects create correlations that limit the domain of validity. We will detail this in the next subsection.

Experimentally, inverse maps can be found from sufficient knowledge of their forward counterparts. Since we are considering finite-dimensional environments, the evolution will have Poincaré recurrences in it. The recurrence time gets longer as the environment gets larger. The evolution of a system state of N dimensions can always be modelled with an environment with N^2 dimensions with a time-dependent Hamiltonian.[42] This makes the number of parameters finite and the problem tractable. A related way to determine the inverse maps to know its forward counterpart to high enough orders in time. Such as scheme for a one-qubit system coupled to a one-qubit environment was developed in Ref. 43. There a finite number of derivatives at the initial time almost fully characterize the evolution of the total state.

In realistic circumstances, full knowledge of the map may not be accomplished. In Sec. 5.5, we will show how incomplete knowledge of the evolution leads to irreversibility. For now, we use the inverse map to derive the canonical dynamical map that accounts for correlations with the environment.

3.3. *Canonical dynamical map*

With the inverse map $\tilde{\mathbb{B}}$, we can now define a *canonical dynamical map* $\mathbb{B}^{\mathsf{C}}$ for states with initially environmental correlations. The knowledge necessary for finding the

[c] The compatibility domain was first introduced to describe system states compatible with initial correlations with their environment.[33,40] Outside the compatibility domain, the positivity of the density matrix need not be preserved by the inverse map. Here we used the term in more general form.

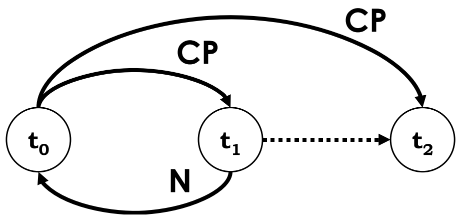

Fig. 1. This diagram represents the evolution described by Eq. (9). **CP** is completely positive evolution, **N** is not positive evolution. A canonical dynamical map from $t_1 \rightarrow t_2$ can be defined going to t_0, and from there forward to t_2, as in Eq. (10).

inverse map are the additional variables needed to extend a system space of a non-Markovian evolution.

We compose the maps to find the evolution described in Eq. (9) from $t_1 \rightarrow t_2$ as in Fig. 1. First, we map the state from t_1 to t_0 using the inverse map, then evolve the state forward to t_2. We write this as

$$\mathbb{B}^{\mathsf{C}}_{(t_2|t_1)} \equiv \mathbb{B}_{(t_2|t_0)} \star \tilde{\mathbb{B}}_{(t_0|t_1)}. \tag{10}$$

The composition is easily computed in the tensor form of the map. From Eq. (10), the canonical dynamical maps have the composition property:

$$\mathbb{B}^{\mathsf{C}}_{(t_f|t_i)} = \mathbb{B}^{\mathsf{C}}_{(t_f|t)} \star \mathbb{B}^{\mathsf{C}}_{(t|t_i)}, \tag{11}$$

without need of any approximations.

It has been implied that $t_0 < t_1 < t_2$, but this need not be. If $t_1 = t_0$, the original completely positive map is obtained. If $t_0 \leq t_1$ but $t_2 = t_0$, we obtain

$$\mathbb{B}^{\mathsf{C}}_{(t_0|t_1)} = \mathbb{B}_{(t_0|t_0)} \star \tilde{\mathbb{B}}_{(t_0|t_1)} = \tilde{\mathbb{B}}_{(t_0|t_1)}, \tag{12}$$

using $\mathbb{B}_{(t_0|t_0)} = \mathbb{I}$, where $\mathbb{I}$ is the identity map. Since $\mathbb{B}^{\mathsf{C}}_{(t_i|t_f)} \star \mathbb{B}^{\mathsf{C}}_{(t_f|t_i)} = \mathbb{B}^{\mathsf{C}}_{(t_f|t_i)} \star \mathbb{B}^{\mathsf{C}}_{(t_i|t_f)} = \mathbb{I}$, we conclude that inverse maps are canonical maps. Canonical maps have the composition property from Eq. (11) and have an inverse from Eq. (12), forming a parameter group in time, also known as an evolution family. They preserve the trace and Hermiticity, but they are in general not positive and are only valid within their compatibility domain. This is what we wanted: A map that allows for correlations with the environment such that any incompatible state with the correlations will give an unphysical total state. If we had full knowledge of the time dependence of the canonical dynamical map, it would be fully irreversible. Only some canonical maps $\mathbb{B}^{\mathsf{C}}_{(t'|t)}$, such as the unitary map, might be completely positive for any choice of t and t'. Another important property is that the derivative of the canonical dynamical map is also well defined for all times, which we will study in Sec. 4.

The canonical dynamical map we have defined describe the most general dynamics of an open quantum systems without the need for the Markov approximation. In the next part, we show the connection between the total unitary dynamics of the system–environment correlations can be described by a canonical embedding map with reduced dynamics given by the canonical dynamical map.

3.4. *Canonical embedding map*

The canonical dynamical map describes the reduced evolution of the system and the environment. To go from the reduced system state, to the total evolution we need to invert the trace at all times. We had described an embedding map $\mathbb{E}_{t_i}$ that could consistently invert the trace map $\mathbb{T}$ for states uncorrelated at time t_i. For clarity, we will focus only on the embedding from Eq. (7) for initially uncorrelated states. Even so, this procedure also work for any valid embedding (completely positive or not completely positive) such as the ones proposed by Pechukas[31] and Alicki.[38] With the use of the canonical map, we can generalize these embedding maps to *all* times, even when the initial correlations have evolved, such that:

$$\eta(t) \to \mathbb{E}_t^{\mathsf{C}} \eta(t) = \rho(t) \quad \text{for all } t. \tag{13}$$

Such an embedding map will use the history of the reduced evolution to close the open system. We evolve the state backwards to the time where we had defined a valid embedding map, undo the trace, and unitarily go forward. From Eq. (5), this would be pictorially represented by

$$\begin{array}{ccccc} & & \mathbb{U}_{(t|t_0)} & & \\ & \rho(t_0) & \Rightarrow & \rho(t) = \mathbb{E}_t^{\mathsf{C}} \eta(t) & \\ \mathbb{E}_{t_0} & \Uparrow & & \uparrow & \\ & \eta(t_0) & \Leftarrow & \eta(t). & \\ & & \mathbb{B}^{\mathsf{C}}_{(t_0|t)} & & \end{array} \tag{14}$$

This *canonical embedding map* from $\eta(t) \to \rho(t)$ is defined as

$$\mathbb{E}_t^{\mathsf{C}} \equiv \mathbb{U}_{(t|t_0)} \star \mathbb{E}_{t_0} \star \mathbb{B}^{\mathsf{C}}_{(t_0|t)}. \tag{15}$$

The canonical embedding map preserves Hermiticity and trace, but might not be positive. Its compatibility domain corresponding to the system space compatible with the correlations existing at time t. The set of states that will give unphysical evolutions is also incompatible with the memory effects of the environment.

We do not demand only an embedding map for uncorrelated total states at t_0; any valid embedding for any other time t will do. The proof for this statement is

$$\begin{aligned} \mathbb{E}_t^{\mathsf{C}} &= \mathbb{U}_{(t|t_0)} \star \mathbb{E}_{t_0} \star \mathbb{B}^{\mathsf{C}}_{(t_0|t)}, \\ &= \mathbb{U}_{(t|t')} \star \left(\mathbb{U}_{(t'|t_0)} \star \mathbb{E}_{t_0} \star \mathbb{B}^{\mathsf{C}}_{(t_0|t')}\right) \star \mathbb{B}^{\mathsf{C}}_{(t'|t)}, \\ &= \mathbb{U}_{(t|t')} \star \mathbb{E}_{t'} \star \mathbb{B}^{\mathsf{C}}_{(t'|t)}. \end{aligned} \tag{16}$$

By knowing one embedding map for a time t' and the unitary operator in the interval $[t, t']$, any other embedding for another t can be found.

This approach explicitly shows the connection between the correlations of the state with the environment and its history. Correlations at one time can be changed to correlations at another as long as the history is known. The necessity of additional knowledge to establish an embedding map plays the role of the additional information, the memory, of a non-Markovian process. The possible negativity of the map shows that the history limits some of the states in the system space to be compatible with the total system−environment state.[9] On the other hand, detailed knowledge of the reduced dynamics can be used to find the full dynamics.[43] The embedding map will be used as a mathematical device to connect the full dynamics to those of the reduced space without the need of the Markov approximation. This connection between system−environment correlations and non-Markovian effects suggests further connections between different witnesses of non-Markovianity and of initial correlations.[18,37,44–47]

3.5. *Classical and quantum correlations as types of non-Markovian dynamics*

The embedding map extends a system state into a system−environment state. As shown in Ref. 9, if the total state has classical correlations, according to quantum discord, the embedding map will in general have positive semidefinite eigenvalues. It was also shown there that if the total state has quantum correlations, the map might have negative eigenvalues. Due to the relationship between the canonical dynamical map and the embedding map from Eq. (6), and since both the trace map and the unitary map are completely positive, it is the eigenvalues of the embedding map that could make the dynamics be noncompletely positive. Since it is these correlations that serve as the memory of the non-Markovian canonical dynamical map, a connection can be drawn where quantum maps can have classical or quantum memory effects according to quantum discord.

In the next section, we show how the derivative of the canonical dynamical map is related to the embedding map.

4. Non-Markovian Master Equation

The non-Markovian master equation can be derived from the canonical dynamical map from Eq. (10). A time derivative of a canonical dynamical map that is non-Markovian must take into account the memory of the process.[48] To consistently obtain a time derivative of the canonical map, we use the property that the time derivative of the unitary operator is $\dot{U} = -iHU$. Since the underlying unitary evolution is always bijective, we can define the time derivative of the canonical map such that:

$$\frac{\partial}{\partial t}\mathbb{B}^{\mathsf{C}}_{(t|t_i)}(\eta(t_i)) = -i\mathrm{Tr}_{\mathcal{E}}[HU_{(t|t_i)}\rho(t_i)U^{\dagger}_{(t|t_i)}] + i\mathrm{Tr}_{\mathcal{E}}[U_{(t|t_i)}\rho(t_i)U^{\dagger}_{(t|t_i)}H]. \tag{17}$$

This is equivalent to a von Neumann equation of the reduced system space, $\mathrm{Tr}_{\mathcal{E}}[\dot{\rho}(t)] = -i\mathrm{Tr}_{\mathcal{E}}[H, \rho(t)]$. To show how the differential equation can explicitly depend only on the system space, we use the embedding map $\mathbb{E}_t^{\mathsf{C}}$ from Eq. (15). The differential equation is

$$\frac{\partial}{\partial t}\eta(t) = -i\mathrm{Tr}_{\mathcal{E}}[H, \mathbb{E}_t^{\mathsf{C}}(\eta(t))]. \tag{18}$$

Now, we write the total Hamiltonian as $H = H_O + H_I$, where H_O is the local (system) part of the Hamiltonian. This local part acts through the embedding map leaving it unchanged. With this, we have the standard form of the non-Markovian master equation:

$$\frac{\partial}{\partial t}\eta(t) = -i[H_O, \eta(t)] + \mathbb{K}_t(\eta(t)), \tag{19}$$

with $\mathbb{K}_t(\cdot) \equiv \mathbb{F}_t(\cdot) + \mathbb{F}_t^{\dagger}(\cdot)$, where

$$\mathbb{F}_t(\cdot) = -i\mathrm{Tr}_{\mathcal{E}}[H_I \mathbb{E}_t^{\mathsf{C}}(\cdot)], \quad \mathbb{F}_t^{\dagger}(\cdot) = +i\mathrm{Tr}_{\mathcal{E}}[\mathbb{E}_t^{\mathsf{C}}(\cdot)H_I]. \tag{20}$$

The embedding map here is just a mathematical device that allows us to show that the Hermitian super operator $\mathbb{K}_t$ is related to the time derivative of the canonical dynamical map by

$$\frac{\partial}{\partial t}\mathbb{B}^{\mathsf{C}}(\cdot) = -i[H_O, \cdot] + \mathbb{K}_t(\cdot). \tag{21}$$

The H_O term is the Hamiltonian evolution of the system and $\mathbb{K}_t$ carries all the effects of the environment, including dissipation and memory.

Since the environment is finite-dimensional, there will be some quasi-periodicity to this evolution as information goes from the system to the environment, and back. At certain times the space is being contracted, while at others it is expanded. These Poincaré recurrences are a consequence of the canonical maps forming a group. This should be contrasted to the Kossakowski–Lindblad master equation, that uses the Markov approximation to obtain a dynamical semigroup.

The Markovian master equation can be obtained by rescaling $\mathbb{K}_t$ to be time independent. The Kossakowski–Lindblad master equation for a process may be obtained by taking the Markov approximation of the dynamical map of that process. From this approximation, irreversibility is introduced. In some cases of this, relaxation into thermodynamic equilibrium can be obtained. Exponential decays are natural solutions to many instances of this equation.

However, the non-Markovian master equation from Eq. (21) allows us to know the full evolution of the system without irreversibility. Thermodynamic effects can be introduced by expanding $\mathbb{K}_t$ for short times without the need of the Markov approximation. As larger orders in time are introduced to the approximation, longer memory effects and higher order correlations with the environment appear. Higher orders in time allow us to go beyond the thermodynamic regime; nonequilibrium quantum thermodynamical effects can be studied. We illustrate this with an example.

5. Example: Qubit System and Qubit Environment

5.1. *Dynamical map*

To illustrate the relationship between the different forms of the map, we compute a simple example of a two-level system, a qubit, represented by the Bloch vector **a**. Its most general transformation in the affine form[49] is

$$\mathbf{a}(t_f) = \overline{R}_{(t_f|t_i)} \cdot \mathbf{a}(t_i) + \mathbf{r}, \tag{22}$$

where the matrix $\overline{R}$ squeezes and rotates the Bloch vector, and the vector **r** translates. In this example, we focus on the particular case where the system interacts with a two-level uncorrelated environment $\tau = \frac{1}{2}\mathbb{I}$. The total initial state is

$$\rho(t_0)^{\mathcal{SE}} = \frac{1}{2}(\mathbb{I}^{\mathcal{S}} + a_j(t_0)\sigma_j^{\mathcal{S}}) \otimes \frac{1}{2}\mathbb{I}^{\mathcal{E}}, \tag{23}$$

where summation over the repeated index j is implied, and σ_j are the Pauli spin matrices. The system $\mathcal{S}$ is described by the Bloch vector **a**. The environment at the initial time is fully mixed. If we assume a unitary operator that depends on the Hamiltonian $H = \sum_j \frac{1}{2}\sigma_j^{\mathcal{S}} \otimes \sigma_j^{\mathcal{E}}$, the evolution of the Bloch vector is

$$\mathbf{a}(t) = \cos{(t-t_0)}^2 \ \mathbf{a}(t_0), \tag{24}$$

which is a uniform shrinking or enlargement of the Bloch sphere with no translation.[50] This interaction was chosen because it swaps the system with the environment at periodic intervals, thus storing the system information in the environment and then returning it. As time changes, the state is pinned to the fully mixed state and grows again into the full state periodically.

The evolution can be treated as a map from $\eta(t_0) \rightarrow \eta(t)$ with the form from Eq. (4). If the density matrix $\eta(t) = \frac{1}{2}(\mathbb{I} + a_j(t)\sigma_j)$ is written as a vector,

$$\boldsymbol{\eta}(t) = \frac{1}{2}\begin{pmatrix} 1 + a_3(t) \\ a_1(t) - ia_2(t) \\ a_1(t) + ia_2(t) \\ 1 - a_3(t) \end{pmatrix}, \tag{25}$$

the evolution is a stochastic matrix transformation $\boldsymbol{\eta}(t) = \mathbb{A}_{(t|t_0)} \cdot \boldsymbol{\eta}(t_0)$, where

$$\mathbb{A}_{(t|t_0)} = \frac{1}{2}\begin{pmatrix} 1+c^2 & 0 & 0 & 1-c^2 \\ 0 & 2c^2 & 0 & 0 \\ 0 & 0 & 2c^2 & 0 \\ 1-c^2 & 0 & 0 & 1+c^2 \end{pmatrix}, \tag{26}$$

with $c \equiv \cos(t - t_0)$. In tensor form, $\mathbb{A}$ can be written as $\mathbb{A}_{rs,r's'}$ where the two indaces rs label each row, while $r's'$ label each column. This $\mathbb{A}$ form of the map was shown in Ref. 1 to be related to the familiar map $\mathbb{B}$ by a simple index exchange

$\mathbb{B}_{rr',ss'} = \mathbb{A}_{rs,r's'}$, such that:

$$\mathbb{B}_{(t|t_0)} = \frac{1}{2}\begin{pmatrix} 1+c^2 & 0 & 0 & 2c^2 \\ 0 & 1-c^2 & 0 & 0 \\ 0 & 0 & 1-c^2 & 0 \\ 2c^2 & 0 & 0 & 1+c^2 \end{pmatrix}. \tag{27}$$

For a detailed example of how to go from $\mathbb{A}$ form to $\mathbb{B}$ form, see Ref. 27. By rewriting the map in terms of its eigenvalues and eigenmatrices, $\eta(t) = \sum_{\alpha=0}^{3} \lambda_\alpha(t-t_0) \times \mathrm{C}_\alpha \eta(t_0) \mathrm{C}_\alpha^\dagger$ with

$$\begin{aligned} \lambda_0(t-t_0) &= \frac{1}{2}(1+3c^2), \quad C_0 = \frac{1}{\sqrt{2}}\mathbb{I}, \\ \lambda_{1,2,3}(t-t_0) &= \frac{1}{2}(1-c^2), \quad\ C_{1,2,3} = \frac{1}{\sqrt{2}}\sigma_{1,2,3}, \end{aligned} \tag{28}$$

we confirm that it is completely positive and trace preserving.

The process is reversible. Since the environment is finite dimensional, there are Poincaré recurrences. Also, note that even if this map is expanded in a Taylor series for $t \approx t_0$, where

$$c^2 = \cos(t-t_0)^2 = 1 - (t-t_0)^2 + \cdots, \tag{29}$$

there are no terms of first order. To get irreversibility from this example, we will need to perform an approximation. In the next section, we review the approximations necessary to obtain the Kossakowski–Lindblad master equation.

5.2. *Kossakowski–Lindblad master equation*

To illustrate the approximations made to obtain the Kossakowski–Lindblad master equation, we study an example. We derive a thermodynamic decay from the collision model developed by Rau.[51] Consider the evolution that leads to Eq. (24). We can model decoherence by treating the total environment as a stream of $\{\tau_i\}$, where each of them interact sequentially for a short average time T. This corresponds to acting with the dynamical map from Eq. (27) in sequence:

$$\eta^{\mathcal{S}} \to \mathbb{B}_{(t_n,t_{n-1})} \star \mathbb{B}_{(t_{n-1},t_{n-2})} \star \cdots \star \mathbb{B}_{(t_1,t_0)}(\eta^{\mathcal{S}}), \tag{30}$$

where each time interval has duration $T = t_m - t_{m-1}$. After N interactions the total time $t = NT$ has passed and the density matrix has the form:

$$\eta(t) = \frac{1}{2}(\mathbb{I}^{\mathcal{S}} + \cos(T)^{2N} a_j(t_0)\sigma_j^{\mathcal{S}}). \tag{31}$$

The shrinking factor can be rewritten as

$$\cos(T)^{2N} = e^{-t\frac{2}{T}\ln\left(\frac{1}{\cos(T)}\right)}. \tag{32}$$

To get a fully thermodynamic decay, we must rescale the short time regime T such that $\frac{2}{T}\ln(\frac{1}{\cos(T)}) \approx \gamma$, where γ is a constant. This rescaling gives an exponential decay of the form:

$$\eta(t) = \frac{1}{2}(\mathbb{I}^{\mathcal{S}} + e^{-\gamma(t-t_0)}a_j(t_0)\sigma_j^{\mathcal{S}}). \tag{33}$$

This evolution can be written as a first-order differential equation, $\dot{\eta}(t) = \gamma(\frac{1}{2}\mathbb{I} - \eta(t))$. If we choose $\mathrm{L}_0 = \sqrt{\frac{\gamma}{3!}}\mathbb{I}$ and $\mathrm{L}_\alpha = \sqrt{\frac{\gamma}{3!}}\sigma_\alpha$ for $\alpha > 0$, the differential equation is of the Kossakowski−Linblad form.

5.3. *Canonical dynamical map and embedding*

We continue the example to illustrate how to compute an inverse map, then the canonical dynamical map and the embedding map. We want to map the Bloch vector $\mathbf{a}$ from the final time t_f to the initial time t_i. In its affine form this is: $\mathbf{a}(t_i) = \overline{R}^{-1}_{(t_f|t_i)} \cdot (\mathbf{a}(t_f) - \mathbf{r})$. For the particular example from Eq. (24), $\mathbf{a}(0) = \frac{1}{c^2}\mathbf{a}(t)$. The inverse $\tilde{\mathbb{A}}_{(t_0|t)}$ can be found from the dynamics,

$$\tilde{\mathbb{A}}_{(t_0|t)} = \frac{1}{2}\begin{pmatrix} 1+c^{-2} & 0 & 0 & 1-c^{-2} \\ 0 & 2c^{-2} & 0 & 0 \\ 0 & 0 & 2c^{-2} & 0 \\ 1-c^{-2} & 0 & 0 & 1+c^{-2} \end{pmatrix}. \tag{34}$$

By index exchange, we obtain $\tilde{\mathbb{B}}_{(t_0|t)}$, which in the eigensystem representation is

$$\begin{aligned} \lambda_0(t-t_0) &= \frac{1}{2}(1+3c^{-2}), \quad \mathrm{C}_0 = \frac{1}{\sqrt{2}}\mathbb{I}, \\ \lambda_{1,2,3}(t-t_0) &= \frac{1}{2}(1-c^{-2}), \quad \mathrm{C}_{1,2,3} = \frac{1}{\sqrt{2}}\sigma_{1,2,3}. \end{aligned} \tag{35}$$

For certain values of t, $\tilde{\mathbb{B}}$ is not completely positive. This represents the periodic behavior of the original map: as the state is squeezed, the compatibility domain of its inverse maps also shrinks. For the times where $c = 0$, the only compatible state is the center of the Bloch sphere. States outside the compatibility domain are not relevant to the physical dynamics of the open system. They are inconsistent with the developed correlations and history.

We can define the canonical dynamical map by means of Eq. (10). The composition property is easier to apply on the $\mathbb{A}$ form of the map, since it is matrix multiplication. We compute $\mathbb{A}_{(t'|t_0)} \cdot \tilde{\mathbb{A}}_{(t_0|t)} = \mathbb{A}_{(t'|t)}$, then exchange the indices to obtain the $\mathbb{B}^{\mathsf{C}}$ form of the canonical map, that has as its eigensystem:

$$\begin{aligned} \lambda_0(t'-t) &= \frac{1}{2}\left(1+3\frac{c^2}{\tilde{c}^2}\right), \quad C_0 = \frac{1}{\sqrt{2}}\mathbb{I}, \\ \lambda_{1,2,3}(t'-t) &= \frac{1}{2}\left(1-\frac{c^2}{\tilde{c}^2}\right), \quad C_{1,2,3} = \frac{1}{\sqrt{2}}\sigma_{1,2,3}, \end{aligned} \tag{36}$$

where $c \equiv \cos(t' - t_0)$ and $\tilde{c} \equiv \cos(t - t_0)$. With $t = t_0$ the map is completely positive. Taking $t' = t$ gives the inverse map.

Finally, a canonical embedding map can be computed from Eqs. (7), (15) and (35):

$$\mathbb{E}_t^{\mathsf{C}}(\eta(t)) = U_{(t|t_0)}([\mathbb{B}^{\mathsf{C}}_{(t_0|t)}(\eta(t))] \otimes \tau)U^{\dagger}_{(t|t_0)}. \tag{37}$$

From Eq. (23), with $\eta(t) = \frac{1}{2}(\mathbb{I} + a_j(t)\sigma_j)$ and $\tau = \frac{1}{2}\mathbb{I}$, we carry out the calculation to reach the final result:

$$\begin{aligned}\mathbb{E}_t^{\mathsf{C}}(\eta(t)) = \ & \frac{1}{4}[\mathbb{I} \otimes \mathbb{I} + a_j(t)(\sigma_j \otimes \mathbb{I} + \tan(t)^2 \mathbb{I} \otimes \sigma_j \\ & + \tan(t)(\sigma_k \otimes \sigma_l - \sigma_l \otimes \sigma_k))],\end{aligned} \tag{38}$$

summing over index j, with $\{j, k, l\}$ being cyclic. The compatibility domain is represented here by the unbounded character of $\tan(t)$. Periodically the compatible set of vectors $\mathbf{a}(t)$ tend to the center of the Bloch sphere. The compatible system parameters change periodically with the correlations.

5.4. *Non-Markovian master equation*

We now illustrate the consistency of Eq. (21). In this case, $H_O = 0$, $H_I = \frac{1}{2} \times \sum_j \sigma_j \otimes \sigma_j$ and $\mathbb{E}_t^{\mathsf{C}}(\eta(t))$ was calculated in Eq. (38). In this case, $\mathbb{F}_t$ from Eq. (20) becomes

$$\mathbb{F}_t(\eta(t)) = \sum_j \frac{1}{4}(-i\tan(t)^2 - 2\tan(t))a_j(t)\sigma_j. \tag{39}$$

The non-Markovian master equation is then:

$$\dot{\eta}(t) = \mathbb{K}_t(\eta(t)) = -\sum_j \tan(t)a_j(t)\sigma_j = 2\tan(t)(\mathbb{I} - 2\eta(t)). \tag{40}$$

If we only look at the σ_j component, the evolution of its expectation value is

$$\dot{a}_j(t) = -2\tan(t)a_j(t), \tag{41}$$

and has as solution $a_j(t) = \cos(t - t_0)^2 a_j(t_0)$. This which agrees with the starting point from Eq. (24).

This is an example of how the total evolution and the non-Markovian dynamical map are related to each other. Similarly, if we know the first derivative of the evolution, as in Eq. (40), partial knowledge of the multiplication of H_I and $\mathbb{K}_t$ can be determined from Eq. (20). Higher derivatives of the canonical map may yield even more information of the full dynamics. Note that there is no dissipation in this equation because we allow for Poincaré recurrences. The role of system–environment correlations is taken care of by Eq. (38).

5.5. *Dissipation beyond the Markov approximation*

The master equation from the example in Sec. 5.4 is not only non-Markovian, it is also periodic. To introduce some dissipation and decay, we must make an approximation for short times in the master equation. Now only memory effects of a small order in time will be kept as the approximation discards some knowledge of the evolution. Irreversibility arise from the limited information.

Experimentally, limited information comes from monitoring the system for only time shorter than Poincaré time, and trying to find the master equation from this incomplete information. It can also come from knowing the dynamics of the reduced system to a limited number of derivatives only.

We approximate $\tan(t) \approx t$ and Eq. (40) becomes:

$$\dot{\eta}(t) = 2t(\mathbb{I} - 2\eta(t)). \tag{42}$$

The evolution of just one component is, $\dot{a_j}(t) = -2t\, a_j(t)$. The solution to this differential equation is

$$a_j(t - t_0) = e^{-(t-t_0)^2} a_j(t_0). \tag{43}$$

As time goes to infinity, the polarization of the Bloch vector shrinks to zero through a nonexponential decay due to the short time memory effects retained from the environment. In other words, the environment is not an ideal (passive) thermodynamic bath as it is dynamically allowed to react slightly. This is an example of a nonequilibrium quantum thermodynamical effect. The decay of the form e^{-t^2} from Eq. (43) should be contrasted to the thermodynamic decay $e^{-\gamma t}$ from Eq. (33). The nonequilibrium thermodynamic decay can be faster than exponential for very small values of γ, while it can be slower for large values of γ. At intermediate values, $\gamma \approx 1$, the non-Markovian decay is slower than exponential at first, and then much faster. Accounting for memory effects and/or correlations of the system to its environment can make decays faster or slower.

The non-Markovian decay also differs from exponential decay close to the initial time. In this nonequilibrium thermodynamic solution, the initial time derivative of the polarization is zero, which is crucial to obtaining the quantum Zeno effect.[23] Before, quantum Zeno could be obtained only from the Hamiltonian part of the Kossakowski−Lindblad master equation. Now, even the interaction with the environment can give rise to a Zeno region.

6. Discussion and Conclusion

We have developed a generalized non-Markovian dynamical map for open quantum systems by accounting for correlations with the environment. Previous work on completely positive non-Markovian master equations can be treated as special classes of the non-Markovian master equation in this paper. For example, Shabani and Lidar[24] proposed a class of master equations whose memory comes from total states with correlations derived from measurement approach. This is equivalent to having an embedding map from Eq. (16) for the particular time t' given by a measurement on the environment. From this, a canonical embedding equation can be developed for all times, and their master equation obtained. This class of embedding is completely positive, at the expense of limiting to only classical correlations of the environment with the system at time t'.[35] Our approach permits any kind of correlations, classical or quantum.

In conclusion, we have discussed how not completely positive dynamical maps in open quantum systems represent the limited domain due to correlations with the environment. With this, a canonical dynamical map was developed that can be applied for any initially correlated systems. The canonical dynamical maps form a dynamical group, different from the dynamical semigroup from the Kossakowski–Lindblad equation. A canonical embedding map can be constructed to express the correlations with the environment at any time, effectively closing the evolution of the open system. A generalized non-Markovian master equation was constructed that was local in time and corresponds to the reduced space von Neumann equation. Approximations to this equation, such as the ones given by a limited knowledge of the history, or knowledge of the evolution of the system to a small order in time, can lead to irreversible behavior beyond the purely thermodynamic regime. This theory permits the study of nonequilibrium quantum thermodynamic effects.

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