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Completely positive maps and classical correlations

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Abstract

We expand the set of initial states of a system and its environment that are known to guarantee completely positive reduced dynamics for the system when the combined state evolves unitarily. We characterize the correlations in the initial state in terms of its quantum discord [1]. We prove that initial states that have only classical correlations lead to completely positive reduced dynamics. The induced maps can be not completely positive when quantum correlations including, but not limited to, entanglement are present.

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1. Introduction

In the mathematical theory of open quantum systems [2] it is often assumed that the system of interest and its environment are initially in a product state. This restrictive assumption precludes the theory from describing a wide variety of experimental situations including that in which an open system is simply observed for some interval of time without attempting to initialize it in any particular state at the beginning of the observation period. If dynamical maps [3] are used to describe the open evolution, then an initial product state would lead to dynamics of the system described in terms of completely positive maps [4, 5]. There has been significant experimental and theoretical interest in quantum correlations, entanglement and coherence in the context of quantum information theory [6]. It is only recently that interest has picked up in investigating how these properties, when present in the initial state of a system and its environment, affects the open evolution of the system [7–14].

Imagine that the time evolution of a state of a system that is open to its environment is observed and found to be completely positive. What does this say about the relationship between the system and its environment at the start of the quantum process? From the observed evolution is it possible to conclude that the two were initially in a product state? In this paper, we investigate the question of how to relax the initial product state assumption and still obtain dynamics for the system that are described by completely positive transformations. We find that the system and its environment can initially be in a more complicated state than a product and certain restricted types of correlations between the two will not destroy the complete positivity of the reduced system dynamics.

Consider a generic finite-dimensional bipartite state $\rho^{\mathcal{SE}}$ of a quantum system $\mathcal{S}$ and its environment $\mathcal{E}$. Unitary evolution of $\rho^{\mathcal{SE}}$ induces a transformation on the system that is described by a trace-preserving Hermitian superoperator called a dynamical map $\mathfrak{B}$. The dynamical map is defined by

$$\eta \to \mathfrak{B}(\eta) \equiv \mathrm{Tr}_{\mathcal{E}}[U\rho^{\mathcal{SE}}U^{\dagger}] = \eta', \tag{1}$$

where $\eta = \mathrm{Tr}_{\mathcal{E}}\rho^{\mathcal{SE}}$ is the initial state of $\mathcal{S}$ and η' is its final state. By assumption, only the state of the system can be directly observed. The dynamical map is linear; consequently, none of the parameters that determine the state of the system appear in it. On the other hand, parameters that determine the overall state $\rho^{\mathcal{SE}}$ but do not appear in η can appear in the map and they will effectively be identified as parameters that describe the evolution and not the state of the system of interest.

We use η to represent density matrices of the system $\mathcal{S}$ and τ to represent density matrices of the environment. The action of the map can be written in terms of its eigenmatrices $\{\zeta^{(\alpha)}\}$ and eigenvalues $\{\lambda_\alpha\}$,

$$\mathfrak{B}(\eta) = \sum_\alpha \lambda_\alpha \zeta^{(\alpha)} \eta \zeta^{(\alpha)\dagger}. \tag{2}$$

If the initial states of the system and its environment are product states, $\rho^{\mathcal{SE}} = \eta \otimes \tau$, then the eigenvalues of the dynamical map are all positive for any choice of unitary evolution [4, 5]. In this case we can define $C^{(\alpha)} \equiv \sqrt{\lambda_\alpha}\zeta^{(\alpha)}$ to get

$$\mathfrak{B}(\eta) = \sum_\alpha C^{(\alpha)} \eta C^{(\alpha)\dagger}, \tag{3}$$

with $\sum_\alpha C^{(\alpha)\dagger} C^{(\alpha)} = \mathbb{1}$. Any map that can be written in this form is completely positive [15, 16].

Can the dynamical maps formalism still be used if the initial system and environment state is not a product state? Yes, but correlations of the system with the environment mean that a few extra considerations apply. For one, the dynamical map is usually not completely positive and very often not even positive [7]. The not completely positive nature of the map means that only a subset of the set of states of the system gets mapped to other states by the dynamical maps. The dynamical map is well defined if it is positive on a large enough set of states such that it can be extended by linearity to all states of the system. The set of states that get mapped to other states by the map defined for a particular time is called the *positivity domain* corresponding to that time. There is a set of states that get mapped to other states by the map defined at all times. It can be shown that this set of states is precisely those that are *compatible* with the correlations that are assumed to be present in the initial state of the system and the environment [9, 10]. The realization that all the states that get mapped to matrices that do not represent states at some time or the other by the map are precisely those states that were excluded by the correlations that were assumed to be present in the initial combined state removes the problems that were previously thought to be present in giving a physical interpretation to the action of not completely positive maps. We note here that positivity of the map should not be confused with the property of complete positivity. Complete positivity is a property of the *form* of the map (it has positive eigenvalues), while positivity is a property of the *action* of the map (it maps density matrices to density matrices).

Do all correlations in the initial state of the system and the environment lead to not completely positive maps or are there certain kinds of correlations that preserve the complete positivity of the reduced evolution of states of the system? In this paper, we identify a general class of initial states that under *any* unitary transformation induce completely positive reduced dynamics for the system. Simply separable states are of a tensor product form, such as $\rho^{\mathcal{SE}} = \eta \otimes \tau$, are a subset of this general class of states. To characterize this class we use the notion of quantum discord introduced by Ollivier and Zurek [1].

2. Example of a not completely positive map coming from an initial state with no entanglement

Since we know that entanglement in $\rho^{\mathcal{SE}}$ typically leads to not completely positive dynamics for $\mathcal{S}$ [12], we first look to see if separability of the initial state is sufficient to guarantee complete positivity. We find that this is not so and illustrate this with an example that shows how not completely positive dynamics arise in physically realizable situations where the initial state is separable but not a product. Let $\mathcal{S}$ and $\mathcal{E}$ both be qubits in a combined initial state,

$$\rho^{\mathcal{SE}} = \tfrac{1}{4}(\mathbf{1} \otimes \mathbf{1} + a_j\sigma_j \otimes \mathbf{1} - c_{23}\sigma_2 \otimes \sigma_3), \tag{4}$$

where $j = \{1, 2, 3\}, \sigma_j$ are the Pauli matrices, a_j and c_{23} are real, and repeated indices are summed over. The state $\rho^{\mathcal{SE}}$ is separable according to the Peres separability criterion [17]. The initial state of the system is

$$\eta = \mathrm{Tr}_{\mathcal{E}}[\rho^{\mathcal{SE}}] = (\mathbf{1} + a_j\sigma_j)/2.$$

The state η depends on the parameters $\{a_j\}$, which are the components of the Bloch vector such that $||\vec{a}|| \leqslant 1$. Furthermore, η will also be limited by the positivity condition of the *total* state $\rho^{\mathcal{SE}}$, which implies that $\vec{a}$ must be compatible with the value of the parameter c_{23}. All possible values of $\{a_j\}$ that comply with this constraint are said to belong to the compatibility domain [10].

Consider a unitary evolution of $\rho^{\mathcal{SE}}$ given by

$$U = \cos(\omega t)\mathbf{1} \otimes \mathbf{1} - \mathrm{i}\sin(\omega t)\sigma_j \otimes \sigma_j. \tag{5}$$

The state of the system at time *t* is given by [18, 19],

$$\tfrac{1}{2}[\mathbf{1} + \cos^2(2\omega t)a_j\sigma_j + c_{23}\cos(2\omega t)\sin(2\omega t)\sigma_1].$$

The dynamical map $\mathfrak{B}$ that describes the open evolution of the system qubit $\mathcal{S}$ is an affine transformation [20] that squeezes the Bloch sphere of the qubit into a sphere of radius $\cos^2(2\omega t)$ and shifts its center by $c_{23}\cos(2\omega t)\sin(2\omega t)$ in the σ_1 direction. By writing $\mathfrak{B}$ in the form equation (2), we obtain

$$\mathfrak{B} = \frac{1}{2}\begin{pmatrix} 1+C^2 & 0 & c_{23}CS & 2C^2 \\ 0 & 1-C^2 & 0 & c_{23}CS \\ c_{23}CS & 0 & 1-C^2 & 0 \\ 2C^2 & c_{23}CS & 0 & 1+C^2 \end{pmatrix}, \tag{6}$$

where $C \equiv \cos(2\omega t)$ and $S \equiv \sin(2\omega t)$. The eigenvalues of $\mathfrak{B}$ are

$$\lambda_{1,2} = \tfrac{1}{2}[1 - \cos^2(2\omega t) \pm c_{23}\cos(2\omega t)\sin(2\omega t)],$$

$$\lambda_{3,4} = \tfrac{1}{2}\left[1 + \cos^2(2\omega t) \pm \cos(2\omega t)\sqrt{4\cos^2(2\omega t) + c_{23}^2\sin^2(2\omega t)}\right].$$

Note that λ_3 and λ_4 are always positive. For λ_1 and λ_2 to be positive we need $\sin^2(2\omega t) \geqslant \pm c_{23}\cos(2\omega t)\sin(2\omega t)$. We can choose c_{23} such that this condition will be violated for some values of ωt making the map $\mathfrak{B}$ not completely positive and it cannot be written in the form given in equation (3). This example shows that even separable states can lead to not completely positive maps. A similar example has been worked out in [13]. The map $\mathfrak{B}$ has a physical interpretation as long as it is applied to initial states η that are *compatible* with the total state $\rho^{\mathcal{SE}}$ [11]. However, the positivity domain can depend on the particular evolution. In this example, if we take $\omega = 0$ such that the evolution is trivial, the eigenvalues of the map are always positive even though there were initial correlations.

In general, do all correlations lead to not completely positive maps? Is there a way of characterizing these correlations that let us easily see if a given initial state will lead to completely positive dynamics under *any* unitary?

3. Classical correlations and quantum discord

The traditional division of bipartite density matrices ρ^{XY} into separable and entangled is often taken to be synonymous with classical correlations and quantum correlations respectively [21]. Ollivier and Zurek [1] and independently Henderson and Vedral [22] have proposed a different definition for classical and quantum correlations in density matrices based on information theoretic considerations. Suggestions for characterizing the correlations along similar lines were also made by Bennett *et al* in [23, 24].

Correlations in classical information theory between random variables X and Y that describe a probability distribution can be measured by the mutual information

$$\mathbf{J}(\mathsf{Y}:\mathsf{X}) = \mathbf{H}(\mathsf{Y}) - \mathbf{H}(\mathsf{Y}|\mathsf{X}),$$

where $\mathbf{H}$ is Shannon entropy, $\mathbf{H}(\mathsf{Y}|\mathsf{X})$ is the conditional entropy of Y given X. As a consequence of Bayes' rule the conditional entropy can be written as $\mathbf{H}(\mathsf{Y}|\mathsf{X}) = \mathbf{H}(\mathsf{Y},\mathsf{X}) - \mathbf{H}(\mathsf{X})$. This leads to a different but equivalent formula for the classical mutual information

$$\mathbf{I}(\mathsf{Y}:\mathsf{X}) = \mathbf{H}(\mathsf{X}) + \mathbf{H}(\mathsf{Y}) - \mathbf{H}(\mathsf{X},\mathsf{Y}).$$

These definitions have to be reexamined for quantum correlations. Since the information that can be obtained from a quantum system depends on the choice of measurements that are performed on it, the quantum version of the conditional entropy differs from the conditional entropy for classical information. If X and Y are quantum systems with their state described by the density matrix ρ^{XY}, then the conditional entropy of the system Y depends on the outcomes of system X due to a set of measurements made on it. These measurement can be written in terms of a particular set of one-dimensional orthogonal projectors $\left\{\Pi_j^{\mathsf{X}}\right\}$ acting on the space of X. Hence to compute $\mathbf{J}(\mathsf{Y}:\mathsf{X})$, we change the definition of $\mathbf{H}(\mathsf{Y}|\mathsf{X})$ to

$$\mathbf{H}(\mathsf{Y}|\mathsf{X}) = \min_{\{\Pi_j^{\mathsf{X}}\}} \mathbf{H}\left(\mathsf{Y}\middle|\left\{\Pi_j^{\mathsf{X}}\right\}\right),$$

where

$$\mathbf{H}\left(\mathsf{Y}\middle|\left\{\Pi_j^{\mathsf{X}}\right\}\right) = \sum_j p_j \mathbf{H}\left(\rho_{\mathsf{Y}|\Pi_j^{\mathsf{X}}}\right),$$

with $p_j = \mathrm{Tr}_{\mathsf{X},\mathsf{Y}} \Pi_j^{\mathsf{X}} \rho^{\mathsf{XY}}$, $\rho_{\mathsf{Y}|\Pi_j^{\mathsf{Y}}} = \Pi_j^{\mathsf{X}} \rho^{\mathsf{XY}} \Pi_j^{\mathsf{X}}/p_j$, and the Shannon entropy is replaced by the von Neumann entropy. The difference between $\mathbf{I}$ and $\mathbf{J}$ is called *quantum discord* and it is taken as a measure of non-classical correlations in a quantum state [1].

A quantum state with only classical correlations satisfies the condition $\rho^{\mathsf{XY}} = \sum_j \Pi_j^{\mathsf{X}} \rho^{\mathsf{XY}} \Pi_j^{\mathsf{X}}$. States of this form are a subset of the set of all separable states and the subset includes all simply separable (tensor product) states. On the other hand, not all separable states have only classical correlations implying that quantum correlations must be taken to

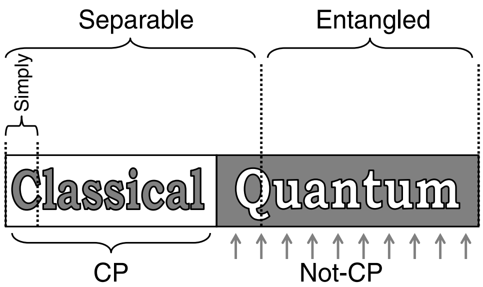

Figure 1. Quantum states of bipartite systems can be divided into having classical and quantum correlations. Separable states can have quantum correlations while simply separable states have only classical correlations. Not all quantum correlations are equivalent to entanglement. Also shown is the nature of the dynamical maps induced by any unitary evolution of the state of a system and its environment when the initial state belongs to each class. Classically correlated states are a sufficient condition for completely positive maps while there are examples, indicated by the arrows, showing that states with quantum correlations can lead to not completely positive maps.

mean more than just entanglement. The information theoretic characterization of quantum states based on the nature of the correlations present is compared with the traditional division into separable and entangled states in figure 1.

Since measurements can be used to initialize quantum states, classically correlated states are of experimental interest. This is done by performing a complete set of (non-selective) orthogonal projective measurements $\{\Pi_j\}$ on the system. After the measurements, the initial state of the system and its environment are *not* uncorrelated, having the form

$$\rho^{\mathcal{SE}} = \sum_j \Pi_j \rho^{\mathcal{SE}} \Pi_j = \sum_j p_j \Pi_j \otimes \tau_j, \tag{7}$$

where τ_j are density matrices for $\mathcal{E}$ and $\{\Pi_j\}$ are a complete set of orthogonal projectors on $\mathcal{S}$, $p_j \geqslant 0$ and $\sum_j p_j = 1$. Sending a beam of photons through a polarizer or an electron beam through a Stern–Gerlach apparatus are examples of this type of preparations. Thus, classically correlated states appear often as the initial state for many quantum processes.

4. Classically correlated states lead to completely positive maps

We now reach the main result of this paper.

Theorem. *Initially classically correlated state of the form* $\rho^{\mathcal{SE}} = \sum_j p_j \Pi_j \otimes \tau_j$ *always lead to completely positive dynamics.*

Proof. We start from the classically correlated state from equation (7) for the system and its environment. The initial state of the system is $\eta = \sum_j p_j \Pi_j$. From equation (1) we have

$$\eta'_{rs} = [\mathfrak{B}]_{rr';ss'} \eta_{r's'} = \mathrm{Tr}_{\mathcal{E}} \left\{ [U]_{ra;r'a'} \left(\sum_j p_j [\Pi_j]_{r's'} [\tau_j]_{a'b'} \right) [U]^*_{sb;s'b'} \right\}.$$

Taking the trace with respect to the environment by contracting indices a and b, we get

$$\eta'_{rs} = \sum_j p_j \left[D_j^{kl}\right]_{rr'} [\Pi_j]_{r's} \left[D_j^{kl}\right]^*_{ss'},$$

where $\left[D_j^{kl}\right]_{rr'} \equiv [U]_{rl;r'a'}[\sqrt{\tau_j}]_{a'k}$. We have used the fact that $\{\tau_j\}$ are positive to take their square root. After combining indices k and l into a single index α, we obtain

$$\eta' = \sum_{j,\alpha} p_j D_j^{(\alpha)} \Pi_j D_j^{(\alpha)\dagger}.$$

Expanding $D_j^{(\alpha)}$ as $\sum_m D_m^{(\alpha)} \delta_{jm}$ and using $\Pi_j^2 = \Pi_j$,

$$\eta' = \sum_{j,\alpha} p_j \left(\sum_m D_m^{(\alpha)} \delta_{jm} \Pi_j \right) \Pi_j \left(\sum_n \Pi_j \delta_{jn} D_n^{(\alpha)\dagger} \right).$$

Now we can use the orthogonality of projectors, $\Pi_m \Pi_j = \delta_{mj} \Pi_j$ to drop the dependence of $D_j^{(\alpha)}$ on index j and write

$$\eta' = \sum_{j,\alpha} p_j \left(\sum_m D_m^{(\alpha)} \Pi_m \right) \Pi_j \Pi_j \Pi_j \left(\sum_n D_n^{(\alpha)} \Pi_n \right)^\dagger.$$

We can redefine $C^{(\alpha)} \equiv \sum_m D_m^{(\alpha)} \Pi_m$ to obtain

$$\eta' = \sum_\alpha C^{(\alpha)} \left(\sum_j p_j \Pi_j \right) C^{(\alpha)\dagger} = \sum_\alpha C^{(\alpha)} \eta C^{(\alpha)\dagger},$$

which is identical to equation (3) showing that it is a completely positive map. This completes the proof. □

Remark. The map $\mathfrak{B}$ comes from the contraction of the unitary evolution of the combined state. Note that by specifying the initial state $\rho^{\mathcal{SE}}$ in equation (7) we have restricted ourselves to the subset of all possible initial system states that is spanned by the projectors $\{\Pi_j\}$. We have shown that the reduced dynamics on these states coming from arbitrary unitary transformations on the extended, classically correlated, state is completely positive. Once the superoperator describing this dynamics has been identified, its action can be extended to all states of the system and the complete positivity of the map guarantees that it will transform physical states to states. For all the states inside the subset spanned by $\{\Pi_j\}$ we have the additional benefit of seeing how the map could arise in a real physical systems. For states outside this subset we do not have the advantage of an obvious mechanism that would explain the action of the map, but all the same the map takes density matrices to density matrices. Our result shows that *any* reduced unitary evolution of an open system that is initially *classically correlated* will be completely positive[3].

The evolution of an open system that has initial quantum correlations with the environment might lead to not completely positive maps as shown in figure 1. We propose that if a not completely positive map is found in an experiment, this should be considered as a signature that the system had quantum correlations with the environment [4].

[3] This result is different from Tong *et al* [25]. They show that a particular initial state can be connected to a particular final state by matrices that have a form similar to equation (3). However, since matrices depend both on the initial and final state, their result has to be interpreted as a point to point connection rather than a map.

[4] Our definition of quantum correlations is different from those considered in previous studies by other authors [13, 14].

5. Example of completely positive map from classical correlations

We can compute an example of completely positive maps coming from a classically correlated state by preparing the state given by equation (4) with a set of projective measurements $\{\Pi_j\}$ along the σ_2 direction on the system space. This gives the initial state $\sum_j \Pi_j \rho^{\mathcal{SE}} \Pi_j = \frac{1}{4}(\mathbf{1} \otimes \mathbf{1} + a_2\sigma_2 \otimes \mathbf{1} - c_{23}\sigma_2 \otimes \sigma_3)$, which is only classically correlated. By evolving this state using the unitaries given by equation (5), the following dynamical map is obtained:

$$\mathfrak{B} = \frac{1}{2}\begin{pmatrix} 1 & 0 & c_{23}CS & C^2 \\ 0 & 1 & -C^2 & c_{23}CS \\ c_{23}CS & -C^2 & 1 & 0 \\ C^2 & c_{23}CS & 0 & 1 \end{pmatrix}, \tag{8}$$

where $C \equiv \cos(2\omega t)$ and $S \equiv \sin(2\omega t)$. Its eigenvalues are

$$\lambda_{1,2} = \tfrac{1}{2}[1 + \sqrt{\cos^4(2\omega t) + (c_{23}\cos(2\omega t)\sin(2\omega t))^2}],$$

$$\lambda_{3,4} = \tfrac{1}{2}[1 - \sqrt{\cos^4(2\omega t) + (c_{23}\cos(2\omega t)\sin(2\omega t))^2}],$$

which are always positive as expected.

6. Identifying correlations using quantum process tomography

It is often assumed that quantum process tomography corresponds to the experimental reconstruction of dynamical maps [6]. A number of known initial states, sufficient to span the space of density matrices of the system, are allowed to evolve as a result of an unknown process. We look at a quantum process tomography experiment on a solid-state qubit performed by Howard *et al* [26, 27] in the light of the results presented above. In this experiment, the system of interest is a qubit formed in a nitrogen vacancy defect in a diamond lattice. The qubit was initialized to the state η_0 with $p_0 = \mathrm{Tr}[|\phi\rangle\langle\phi|\eta_0] = 0.7$. The state is not pure; it cannot be ruled out that the system could be correlated to the environment. The map corresponding to the decoherence process was found to have negative eigenvalues. The not completely positive map found in this experiment could be interpreted as an indication that the initial state of the system is not just classically correlated with the environment. Given that the qubit is in a large crystal lattice, it is perhaps not very surprising that it had quantum correlations with its surroundings. A detailed study of the connection of the evolution of open quantum systems and quantum process tomography can be found in [28].

7. Conclusions

In conclusion, we have studied the effect of initial correlations with the environment on the complete positivity of dynamical maps that describe the open-systems evolution. We proved that classical correlations of the state of the system and its environment, as indicated by zero discord, are a sufficient condition the maps induced by any unitary evolution of the combined state to be completely positive. This result is more general than the previously known result for simply separable initial states, and it is important toward clarifying the boundary between completely positive and not completely positive maps.

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