Completely positive maps and classical correlations

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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 [H. Ollivier and W. H. Zurek, Phys. Rev. Lett. **88**, 017901 (2001)]. 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. We outline the implications of our results to quantum process tomography experiments.

In the mathematical theory of open quantum systems [1, 2, 3] it is often assumed that the system of interest and its environment are initially in a product state. This extremely restrictive assumption precludes the theory from describing a wide variety of experimental situations including the one 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 [4] are used to describe the open evolution, then it is known that an initial product state leads to dynamics of the system described in terms of completely positive maps [5, 6, 7, 8, 9]. There has been significant experimental and theoretical interest in quantum correlations, entanglement and coherence in the context of quantum information theory [10]. 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 [11, 12, 13, 14, 15, 16, 17]. In this Letter we investigate the related question of how to relax the initial product state assumption and still obtain dynamics for the system that are described by completely positive transformations.

Consider a generic bipartite state $\rho^{\mathcal{SE}}$ of a quantum system $\mathcal{S}$ and its environment $\mathcal{E}$. Unitary evolution of the combined state induces transformations on the system state described by a dynamical map $\mathfrak{B}$ defined as

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

where $\eta = \mathrm{Tr}_{\mathcal{E}}\rho^{\mathcal{SE}}$ is the initial state of $\mathcal{S}$ and η' is its final state. We use η to represent density matrices of the system $\mathcal{S}$ and τ to represent density matrices of the environment $\mathcal{E}$. The action of the map can be written in terms of its eigenmatrices $\{\zeta^{(\alpha)}\}$ and eigenvalues $\{\lambda_\alpha\}$,

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

If the initial state of the system and its environment is simply separable (product) so that $\rho^{\mathcal{SE}} = \eta \otimes \tau$, then the eigenvalues of the dynamical map are all positive for any choice of unitary evolution [8, 9]. In this case we can define $C^{(\alpha)} \equiv \sqrt{\lambda_\alpha}\zeta^{(\alpha)}$ to get

$$\mathfrak{B}(\eta) = \sum_\alpha C^{(\alpha)}\eta {C^{(\alpha)}}^{\dagger}, \tag{2}$$

with $\sum_\alpha {C^{(\alpha)}}^{\dagger} C^{(\alpha)} = 1$. Any map that can be written in this form is completely positive [5, 6]. If the initial system and environment state is not a product state, then the map induced by arbitrary unitary evolution on $\rho^{\mathcal{SE}}$ is in general not completely positive [11, 12]. In this Letter we identify a general class of initial states such that *any* unitary transformation on it leads to completely positive reduced dynamics for the system. Simply separable states 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 [18] and independently by Henderson and Vedral [19].

First, we consider an example that shows how not completely positive dynamics arise in physically realizable situations where the initial state is separable but not simply separable. Let $\mathcal{S}$ and $\mathcal{E}$ both be qubits in a combined initial state,

$$\rho^{\mathcal{SE}} = \frac{1}{4}(\mathbb{1}\otimes\mathbb{1} + a_j\sigma_j\otimes\mathbb{1} + c_{23}\sigma_2\otimes\sigma_3), \tag{3}$$

where $j = 1, 2, 3$, σ_j are the Pauli matrices and repeated indices are summed over. To show that $\rho^{\mathcal{SE}}$ is a separable state we use the Peres partial transpose test [20] which is a necessary and sufficient test for entanglement in two qubit systems. The transpose operation takes σ_2 to $-\sigma_2$ while leaving the other two Pauli matrices intact. If we apply the partial transpose test to $\rho^{\mathcal{SE}}$ by transposing $\mathcal{E}$, we see from Eq. (3) that $(\rho^{\mathcal{SE}})^{\mathrm{PT}} = \rho^{\mathcal{SE}}$ and so it is a separable state. The initial state of the system is $\eta = \mathrm{Tr}_{\mathcal{E}}[\rho^{\mathcal{SE}}] = (\mathbb{1} + a_j\sigma_j)/2$.

Consider a unitary evolution of $\rho^{\mathcal{SE}}$ given by $U = e^{-iHt} = \cos(\omega t)\mathbb{1}\otimes\mathbb{1} - i\sin(\omega t)\sigma_j\otimes\sigma_j$, where $H = \omega\sum_j \sigma_j\otimes\sigma_j$. The state of the system at time t is given by [21, 22]

$$\eta' = \frac{1}{2}\big[\mathbb{1} + \cos^2(2\omega t)\, a_j\sigma_j + c_{23}\cos(2\omega t)\sin(2\omega t)\,\sigma_1\big].$$

The dynamical map $\mathfrak{B}$ that describes the open evolution of the system qubit $\mathcal{S}$ is an affine transformation [23] 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. The eigenvalues of the map are

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

It is easily seen that $\lambda_{3,4}$ are always positive, while for $\lambda_{1,2}$ to be positive we need $\sin^2(2\omega t) \geq \pm c_{23}\cos(2\omega t)\sin(2\omega t)$. 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. It has been previously shown that not completely positive maps come from initial entanglement [14]. This example shows that even separable states can lead to not completely positive maps. A similar example has been worked out in [15]. 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 $\rho^{\mathcal{SE}}$ [13].

From this example we see that correlations, and not necessarily entanglement, in the initial state of the system and its environment can lead to not completely positive reduced dynamics for $\mathcal{S}$. Do all correlations lead to not completely positive maps? If not, is there a way of characterizing these correlations that lets us easily see if a given initial state will lead to completely positive dynamics or not?

The traditional division of bipartite density matrices ρ^{XY} into separable ($\rho^{\mathsf{XY}} = \sum_j p_j\eta_j \otimes \tau_j$) and entangled is often taken to be synonymous with classical correlations and quantum correlations respectively [24]. Ollivier and Zurek [18] and independently Henderson and Vedral [19] 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 [25, 26].

To quantify the correlations between two systems X and Y, we can either compute the mutual information,

$$\mathbf{I}(\mathsf{Y}:\mathsf{X}) = \mathbf{H}(\mathsf{X}) + \mathbf{H}(\mathsf{Y}) - \mathbf{H}(\mathsf{X}\cup\mathsf{Y}), \qquad (4)$$

or its classical equivalent,

$$\mathbf{J}(\mathsf{Y}:\mathsf{X}) = \mathbf{H}(\mathsf{Y}) - \mathbf{H}(\mathsf{Y}|\mathsf{X}), \qquad (5)$$

where $\mathbf{H}$ is the Shannon entropy [27]. If X and Y are classical systems in the sense that their states are described by probability distributions over two random variables X and Y, then $\mathbf{J} = \mathbf{I}$ as a consequence of Bayes' rule.

If X and Y are quantum systems with their state described by the density matrix ρ^{XY}, then the mutual information between the two can be computed by replacing the Shannon entropy in Eq. (4) by the von Neumann entropy $\mathbf{H}(\rho) = -\mathrm{Tr}\rho\log\rho$ [28]. To compute $\mathbf{J}(\mathsf{Y}:\mathsf{X})$, the definition of $\mathbf{H}(\mathsf{Y}|\mathsf{X})$ has to be generalized to

$$\mathbf{H}(\mathsf{Y}\big|\{\Pi_j^{\mathsf{X}}\}) = \sum_j p_j \mathbf{H}(\rho_{\mathsf{Y}|\Pi_j^{\mathsf{X}}}), \qquad (6)$$

where $p_j = \mathrm{Tr}_{\mathsf{X},\mathsf{Y}}\Pi_j^{\mathsf{X}}\rho^{\mathsf{XY}}$ and $\rho_{\mathsf{Y}|\Pi_j^{\mathsf{Y}}} = \Pi_j^{\mathsf{X}}\rho^{\mathsf{XY}}\Pi_j^{\mathsf{X}}/p_j$.

Such a generalization is needed because quantum information differs from classical information in that the information that can be obtained from a quantum system depends not only on its state but also on the choice of measurements that is performed on it. So, in generalizing $\mathbf{H}(\mathsf{Y}|\mathsf{X})$, we first had to choose a particular set of one-dimensional orthogonal projectors $\{\Pi_j^{\mathsf{X}}\}$ acting on the system X.

It turns out that for general bipartite quantum states, the mutual information is not identical to $\mathbf{J}(\mathsf{Y}:\mathsf{X})$ defined using Eq. (6). 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 [18].

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 states. On the other hand, not all separable states have only classical correlations. This implies that quantum correlations must be taken to 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 Fig. 1.

In experiments, quantum systems are often initialized in desired states by first performing a complete set of orthogonal projective measurements $\{\Pi_j\}$ on the system and then super-selecting the desired state from the post-measurement state. After the measurements, the initial state of the system and its environment has the form

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

where τ_j are density matrices for $\mathcal{E}$, $\{\Pi_j\}$ are a complete set of orthogonal projectors on $\mathcal{S}$, $p_j \geq 0$ and $\sum_j p_j = 1$.

We now show that initial states of the system and the environment with only classical correlations with respect to the system will always lead to completely positive maps on the system under *any* unitary evolution. Previously, only simply separable states were known to lead to completely positivity reduced dynamics for any choice of unitary evolution for the combined state [15, 17].

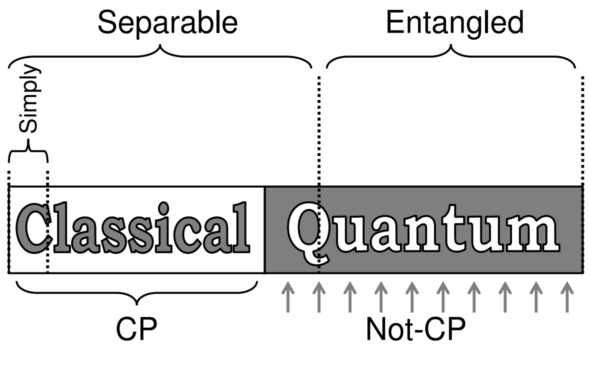

FIG. 1: Quantum states of bipartite systems can be divided into two classes based on their discord. States with quantum correlations have non-zero discord while classically correlated states have zero discord. Separable states can have quantum correlations while simply separable states have only classical correlations. Not all quantum correlations are equivalent to entanglement. Also shown is the nature of the dynamical maps induced by the unitary evolution of the state of a system and its environment when the initial state belongs to each class. Classically correlated states always lead to completely positive (CP) maps while there are examples, indicated by the arrows, showing that states with quantum correlations lead to not completely positive maps (Not-CP).

We start from the classically correlated state from Eq. (7). The initial state of the system is $\eta = \sum_j p_j \Pi_j$. From Eq. (1) we have

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

Take the trace with respect to the environment by contracting indices a and b,

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

where $[D_j^{kl}]_{rr'} \equiv [U]_{rl;r'a'}[\sqrt{\tau_j}]_{a'k}$. 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,

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

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

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

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

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

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

$$\eta' = \sum_\alpha C^{(\alpha)} \Big(\sum_j p_j \Pi_j\Big) C^{(\alpha)\dagger} = \sum_\alpha C^{(\alpha)} \eta C^{(\alpha)\dagger}. \quad (8)$$

Eq. (8) is identical to Eq. (2) showing that $\mathfrak{B}$ indeed is a completely positive map. This demonstrates that *any* reduced unitary evolution of an open system that is initially *classically correlated* with its environment will be given by a completely positive maps. The evolution of an open system that has initial quantum correlations with the environment, on the other hand, might lead to not completely positive maps as shown in Fig. 1.

Note that by specifying the initial state $\rho^{\mathcal{SE}}$ in Eq. (7) we have restricted to a subset of all possible initial system states. This subset is spanned by the projectors $\{\Pi_j\}$. The map $\mathfrak{B}$ from Eq. (8), on the other hand, can be applied to any state of the system. Since the map is completely positive it will map any system state to another valid state. We will not, however, be able to understand the action of the map on states outside the subset spanned by $\{\Pi_j\}$ as coming from the contraction of unitary evolution of the combined state in Eq. (7).

Experimentally reconstructing dynamical maps corresponding to open quantum evolution is called quantum process tomography [10, 29]. 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. The final state corresponding to each initial state is then determined by quantum state tomography. With the knowledge of the initial and corresponding final states the linear dynamical map describing this unknown process is determined. The complete set of initial states for the system is typically generated by creating a fiducial state and then applying controlled evolution on it to obtain the other states. The fiducial state, in turn, is obtained by doing a complete set of orthogonal measurements on the system as described earlier.

We look at a representative quantum process tomography experiment on a solid-state qubit performed by Howard et al. [30, 31] 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. Under ideal conditions, the experiment requires the initial state of the qubit to be the pure state $|\phi\rangle\langle\phi|$, but in reality the qubit is initialized in the state η_0 with $p_0 = \mathrm{Tr}\left[|\phi\rangle\langle\phi|\eta_0\right] = 0.7$.

It is argued in [31] that the population considered was high enough to effectively treat the initial state as $|\phi\rangle\langle\phi|$. From this state a complete set of linearly independent states is constructed stochastically. This provides the set of initial states necessary to perform process tomography on the decoherence occurring to the qubits. The map corresponding to the decoherence process was found and it had negative eigenvalues, making it not completely positive. The experimentally obtained not completely positive maps were then discarded in favor of their "closest" completely positive counterparts [32]. The occurrence of negative eigenvalues for the dynamical maps was attributed to experimental errors.

However, if we do not discard the negative eigenvalues as unphysical, this will yield information about the initial preparation of the system. If the system is indeed in a pure state $\eta_0 \to |\phi\rangle\langle\phi|$ initially then the combined state of the system and its environment would necessarily be of the form $\rho^{\mathcal{SE}} = |\phi\rangle\langle\phi|\otimes\tau$. Maps coming from such initially simply separable states should be completely positive. This contradicts what was found in the experiment. In addition to ruling out an initial simply separable state, we can now also rule out initial states of the form

$$\rho^{\mathcal{SE}} = p_0|\phi\rangle\langle\phi| \otimes \tau' + (1 - p_0)\,|\phi_\perp\rangle\langle\phi_\perp| \otimes \tau'',$$

with $\langle\phi|\phi_\perp\rangle = 0$, even though states of this form are consistent with the measured population p_0. However, a state like this only has classical correlations, and we know that the map induced by any unitary evolution of such a state should be completely positive.

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 the surrounding environment.

We propose that if after performing quantum process tomography a not completely positive map is found, this should be considered as a signature that the system had quantum correlations with the environment. Our definition of quantum correlation is different from the ones considered in other previous studies by other authors [15, 17].

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 if there are only classical correlations in the state of the system and its environment, as indicated by zero discord, then the maps induced by any unitary evolution of the combined state must be completely positive for any unitary transformation. This result is more general than the previously known result for simply separable initial states.

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