Vanishing Quantum Discord is Necessary and Sufficient for Completely Positive Maps

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Two long-standing open problems in quantum theory are to characterize the class of initial system-bath states for which quantum dynamics is equivalent to (i) a map between the initial and final system states, and (ii) a completely positive (CP) map. The CP map problem is especially important, due to the widespread use of such maps in quantum information processing and open quantum systems theory. Here we settle both these questions by showing that the answer to the first is ‘‘all’’, with the resulting map being Hermitian, and that the answer to the second is that CP maps arise exclusively from the class of separable states with vanishing quantum discord.

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Introduction.—Every natural object is in contact with its environment, so its dynamics is that of an ‘‘open’’ system. The problem of the formulation and characterization of the dynamics of open systems in the quantum regime has a long and extensive history [1]. Consider a quantum system S coupled to another system B, with respective Hilbert spaces $\mathcal{H}_S$ and $\mathcal{H}_B$, such that together they form one isolated system, described by the joint initial state (density matrix) $\rho_{SB}(0)$. B represents the environment, or bath, so the object of interest is the system S, whose state at time t is governed according to the standard quantum-mechanical prescription by the following quantum dynamical process (QDP):

$$\rho_S(t) = \mathrm{Tr}_B[\rho_{SB}(t)] = \mathrm{Tr}_B[U_{SB}(t)\rho_{SB}(0)U_{SB}(t)^\dagger]. \quad (1)$$

The propagator $U_{SB}(t)$ is a unitary operator, the solution to the Schrödinger equation $\dot{U}_{SB} = -(i/\hbar)[H_{SB}, U_{SB}]$, where H_{SB} is the joint system-bath Hamiltonian. Tr_B represents the partial trace operation, corresponding to an averaging over the bath degrees of freedom [1].

The QDP (1) is a transformation from $\rho_{SB}(0)$ to $\rho_S(t)$. However, since we are not interested in the state of the bath, it is natural to ask: under which conditions is the QDP a map from $\rho_S(0)$ to $\rho_S(t)$? When is this map linear? When is it completely positive (CP) [1]? These are fundamental questions which have been the subject of intense studies with a long history [2–10]. One reason that these questions have attracted so much interest is the fundamental role played by CP maps in quantum information [11] and open quantum systems theory [1]. CP maps are the ‘‘work-horse’’ in these fields, and hence an understanding of their domain of validity is essential. For this reason it is perhaps surprising that the problem of identifying the general physical conditions under which CP maps are valid has remained open since it was first posed in a vigorous debate [3,4]. In particular, while *sufficient* conditions have been developed for complete positivity [4,10], it is not known which is the most general class of states for which the QDP (1) is always CP, for arbitrary U_{SB}. In this work we settle this old open question. We prove that the QDP yields a CP map $\rho_S(0) \mapsto \rho_S(t)$ iff $\rho_{SB}(0)$ has vanishing ‘‘quantum discord’’ [12], i.e., is purely classically correlated.

In order to arrive at this result we introduce a class of states we call ‘‘special linear’’ (SL), with the property of being of full measure in the set of mixed bipartite states. We show that the QDP (1) is always a linear Hermitian map Φ_H: $\rho_S(0) \mapsto \rho_S(t)$ if $\rho_{SB}(0)$ in the SL class. Vanishing discord states are a subset of SL states, and CP maps are a subset of Hermitian maps; we use the SL construction to prove our main result about CP maps. We then argue that the restriction to the SL class can be lifted, and that in fact the QDP (1) is *always* a linear Hermitian map, for arbitrary $\rho_{SB}(0)$. This result settles another old open question: is quantum subsystem dynamics always a map, and if so, of what kind?

Linear maps.—A linear map is ‘‘Hermitian’’ if it preserves the Hermiticity of its domain. We first present an operator sum representation for arbitrary and Hermitian linear maps:

Theorem 1.—A map Φ: $\mathfrak{M}_n \mapsto \mathfrak{M}_m$ (where $\mathfrak{M}_n$ is the space of $n \times n$ matrices) is linear iff it can be represented as

$$\Phi(\rho) = \sum_\alpha E_\alpha \rho E_\alpha^{\prime\dagger}, \quad (2)$$

where the ‘‘left and right operation elements’’ $\{E_\alpha\}$ and $\{E'_\alpha\}$ are, respectively, $m \times n$ and $n \times m$ matrices.

Φ_H is a Hermitian map iff

$$\Phi_H(\rho) = \sum_\alpha c_\alpha E_\alpha \rho E_\alpha^\dagger, \qquad c_\alpha \in \mathbb{R}. \quad (3)$$

(See Refs. [13,14] for a proof). A linear map is called ‘‘completely positive’’ (CP) if it is a Hermitian map with $c_\alpha \geq 0 \ \forall \ \alpha$. There is a tight connection between CP and Hermitian maps [7,9]: a map is Hermitian iff it can be written as the difference of two CP maps.

The definition of a CP map Φ_{CP} implies that it can be expressed in the Kraus operator sum representation [1]: $\rho_S(t) = \sum_\alpha E_\alpha(t)\rho_S(0)E_\alpha^\dagger(t) = \Phi_{\mathrm{CP}}(t)[\rho_S(0)]$. If the operation elements E_α satisfy $\sum_\alpha E_\alpha^\dagger E_\alpha = I$ then $\mathrm{Tr}[\rho_S(t)] = 1$.

The standard argument in favor of the ubiquitousness of CP maps is that, since S may be coupled with B, the maps $\Phi_{\rm Ph}$ describing physical processes on S should be such that all their extensions into higher dimensional spaces should remain positive, i.e., $\Phi_{\rm Ph} \otimes I_n \geq 0 \quad \forall\ n \in \mathbb{Z}^+$, where I_n is the n-dimensional identity operator; this means that $\Phi_{\rm Ph}$ is a CP map [15]. However, one may question whether this is the right criterion for describing quantum dynamics on the grounds that this imposes restrictions on the allowed class of initial system-bath states [3]. An alternative viewpoint is to seek a description that applies to *arbitrary* $\rho_{SB}(0)$. However, it was recently shown [16] that the QDP (1) with *arbitrary* $\rho_{SB}(0)$ becomes a CP map iff a most restrictive condition is satisfied by $U_{SB}(t)$, namely, it must be locally unitary: $U_{SB}(t) = U_S(t) \otimes U_B(t)$, i.e., the effective system-bath interaction must vanish. If one gives up the consistency condition $\rho_S = {\rm Tr}_B[\rho_{SB}]$ for all ρ_S, or gives up linearity except in the weak coupling regime, CP maps arise for more general initial states [4].

A recent breakthrough due to Rodriguez *et al.* [10] shows that CP maps arise for arbitrary U_{SB} even for certain nonfactorized initial conditions, namely, provided the initial state $\rho_{SB}(0)$ is invariant under the application of a complete set of orthogonal one-dimensional projections on S, i.e., the state has vanishing quantum discord. Here we show that vanishing quantum discord is not only sufficient but also necessary for the QDP to induce a CP map (*Theorem 3*). To this end we first show that the larger class of Hermitian maps is compatible with general initial conditions. (*Theorem 2*).

Special-linear states.—We now define a class of states we call "special-linear" (SL) states for which the QDP (1) always results in a linear, Hermitian map. An arbitrary bipartite state on $\mathcal{H}_S \otimes \mathcal{H}_B$ can be written as

$$\rho_{SB} = \sum_{ij} \varrho_{ij} |i\rangle\langle j| \otimes \phi_{ij}, \tag{4}$$

where $\{|i\rangle\}_{i=1}^{\dim \mathcal{H}_S}$ is an orthonormal basis for $\mathcal{H}_S$, and $\{\phi_{ij}\}_{i,j=1}^{\dim \mathcal{H}_S}$: $\mathcal{H}_B \mapsto \mathcal{H}_B$ are normalized such that if ${\rm Tr}[\phi_{ij}] \neq 0$ then ${\rm Tr}[\phi_{ij}] = 1$. The corresponding reduced system and bath states are then $\rho_S = \sum_{(i,j)\in\mathcal{C}} \varrho_{ij} |i\rangle\langle j|$, where $\mathcal{C} \equiv \{(i,j)|{\rm Tr}[\phi_{ij}] = 1\}$, and $\rho_B(0) = \sum_i \varrho_{ii}\phi_{ii}$. Hermiticity and normalization of ρ_{SB}, ρ_S, and ρ_B imply $\varrho_{ij} = \varrho^*_{ji}$, $\phi_{ij} = \phi^\dagger_{ji}$, and $\sum_i \varrho_{ii} = 1$.

Definition 1.—A bipartite state ρ_{SB} is in the SL class iff either ${\rm Tr}[\phi_{ij}] = 1$ or $\phi_{ij} = 0$, $\forall\ i, j$.

The following is a key result which we prove at the end:

Theorem 2.—If $\rho_{SB}(0)$ is an SL class state then the QDP (1) is a linear, Hermitian map Φ_H: $\rho_S(0) \mapsto \rho_S(t)$.

Next we need to be precise about the block structure associated with a matrix $A = [a_{ij}]$:

Definition 2.—We call two diagonal elements $a_{i_1 i_1}$ and $a_{i_B i_B}$ "block-connected via the path $\{i_b\}_{b=2}^{B-1}$" if there exists a set of unequal indexes $\{i_b\}_{b=1}^{B}$ such that $\{a_{i_b i_{b+1}}\}_{b=1}^{B-1}$ are all nonzero, i.e., they can be connected via a path that involves only horizontal and vertical (but not diagonal) moves. The "block-index set" $\mathcal{D}_A^{(\alpha)}$ is the set of all index pairs $\{(i,j)\}$ of the elements of the αth block of A.

This is just the standard notion of a block in a matrix, possibly before permutation matrices are applied to sort it into the standard block-diagonal structure. We are now ready to state our main result.

Lemma 1.—Let $\rho_{SB}(0)$ [Eq. (4)] be an SL class state, let $\Phi \equiv [\phi_{ij}] = \bigoplus_\alpha \Phi^{(\alpha)}$ (a supermatrix), and let $\{\Pi_\alpha \equiv \sum_{(i,i)\in\mathcal{D}_\Phi^{(\alpha)}} |i\rangle\langle i|\}_\alpha$ be a complete set of projectors from $\mathcal{H}_S$ to $\mathcal{H}_S$. Let $\mathcal{C}_\Phi^{(\alpha)} \equiv \{(i,j) \in \mathcal{D}_\Phi^{(\alpha)} | {\rm Tr}[\phi_{ij}] = 1\}$ and

$$\rho_S^{(\alpha)} \equiv \Pi_\alpha \rho_S(0) \Pi_\alpha / p_\alpha = \sum_{(i,j)\in\mathcal{C}_\Phi^{(\alpha)}} \varrho_{ij} |i\rangle\langle j| / p_\alpha, \tag{5}$$

where $p_\alpha = {\rm Tr}[\rho_S(0)\Pi_\alpha]$. Let $\rho_B^{(\alpha)}$ be a density matrix. The Hermitian map Φ_H: $\rho_S(0) \mapsto \rho_S(t)$ induced by the QDP (1) is a CP map iff $(\Phi^{(\alpha)})_{ij} = \{0 \text{ or } \rho_B^{(\alpha)}\}\ \forall\ (i,j) \in \mathcal{D}_\Phi^{(\alpha)}$:

$$\rho_{SB}(0) = \sum_\alpha p_\alpha \rho_S^{(\alpha)} \otimes \rho_B^{(\alpha)}. \tag{6}$$

Clearly, $\rho_S^{(\alpha)}$ can be thought of as the post-measurement state arising with probability p_α from $\rho_S(0)$ after the application of the projective measurement described by the set $\{\Pi_\alpha\}$. Moreover, $\rho_{SB}(0)$ is not merely separable:

Theorem 3.—The Hermitian map Φ_H: $\rho_S(0) \mapsto \rho_S(t)$ is a CP map iff the initial system-bath state $\rho_{SB}(0)$ has vanishing quantum discord (VQD), i.e., can be written as

$$\rho_{SB}(0) = \sum_{k,\alpha} \Pi_\alpha^k \rho_{SB}(0) \Pi_\alpha^k, \tag{7}$$

where $\{\Pi_\alpha^k\}$ are one-dimensional projectors onto the eigenvectors of $\rho_S^{(\alpha)}$, and $\sum_k \Pi_\alpha^k = \Pi_\alpha$.

Proof.—By expanding $\rho_S^{(\alpha)}$ as $\sum_k p_\alpha^k \Pi_\alpha^k$, with $p_\alpha^k = {\rm Tr}[\rho_S(0)\Pi_\alpha^k] \geq 0$ and $\sum_k p_\alpha^k = 1$, we obtain using Eq. (6): $\rho_{SB}(0) = \sum_\alpha \rho_S^{(\alpha)} \otimes \rho_B^{(\alpha)} = \sum_{k,\alpha} p_\alpha^k \Pi_\alpha^k \otimes \rho_B^{(\alpha)}$, which implies Eq. (7). On the other hand $\sum_{k,\alpha} \Pi_\alpha^k \rho_{SB}(0) \Pi_\alpha^k$ is the state after a nonselective projective measurement $\{\Pi_\alpha^k\}$ on S, so that $\rho_{SB}(0) = \sum_{k,\alpha} p_\alpha^k \Pi_\alpha^k \otimes \rho_B^{(\alpha)}$. ■

The quantum discord has a deep information-theoretic origin and interpretation, for the details of which we refer the reader to Ref. [12]; we shall merely remark that when the discord vanishes all the information about B that exists in the S-B correlations is locally recoverable just from the state of S, which is not the case for a general separable state of S and B. In this sense a VQD state is "completely classical."

Proof of Lemma 1.—We start with necessity; sufficiency will turn out to be trivial. Let us assume that the Hermitian map Φ_H: $\rho_S(0) \mapsto \rho_S(t)$ induced by the QDP, $\rho_S(t) = {\rm Tr}_B[U\rho_{SB}(0)U^\dagger]$, is CP, and determine the class of allowed initial states. We start from an SL class state since we know (*Theorem 2*) that in this case the QDP (1) is indeed equivalent to a Hermitian map. Let $\tilde{M} = |\Psi\rangle\langle\Psi|$, where $|\Psi\rangle = \frac{1}{\sqrt{d_S}}\sum_{i=1}^{d_S}|i\rangle \otimes |i\rangle$ is a maximally entangled state over $\mathcal{H}_S \otimes \mathcal{H}_S$, and where $d_S = \dim\mathcal{H}_S$. It follows directly from Eq. (14) below that $\Phi_H[|i\rangle\langle j|] = \mathrm{Tr}_B[U|i\rangle \times \langle j| \otimes \phi_{ij}U^\dagger]$. Thus the Choi matrix [15] for Φ_L is

$$\mathcal{M} \equiv (I \otimes \Phi_H)[\tilde{M}] = \frac{1}{d_S}\sum_{ij}|i\rangle\langle j| \otimes \Phi_H[|i\rangle\langle j|] = \frac{1}{d_S}\sum_{ij}|i\rangle\langle j| \otimes \mathrm{Tr}_B[U|i\rangle\langle j| \otimes \phi_{ij}U^\dagger]. \tag{8}$$

We assume that $\mathcal{M}$ is positive as this is equivalent to Φ_H being CP [15]. A useful fact is that a matrix A is positive iff every principal submatrix of A is positive (a principal submatrix is the matrix obtained by deleting from A some number of columns and rows with equal indexes). Therefore, let us focus on the pair of rows and columns (k, l) $(k \neq l)$ of $d_S\mathcal{M}$, and consider the 2×2 principal submatrix

$$P_{kl} = \begin{pmatrix} \mathrm{Tr}_B[U|k\rangle\langle k| \otimes \phi_{kk}U^\dagger] & \mathrm{Tr}_B[U|k\rangle\langle l| \otimes \phi_{kl}U^\dagger] \\ \mathrm{Tr}_B[U|l\rangle\langle k| \otimes \phi_{lk}U^\dagger] & \mathrm{Tr}_B[U|l\rangle\langle l| \otimes \phi_{ll}U^\dagger] \end{pmatrix}. \tag{9}$$

The submatrix P_{kl} must be positive for any U, and we choose to examine the case $U = \frac{1}{\sqrt{2}}(I \otimes I - iX \otimes A)$, where A is Hermitian and unitary (hence $A^2 = I$), and $X = |k\rangle\langle l| + |l\rangle\langle k| + \sum_{i\neq k,l}|i\rangle\langle i|$. This will allow us to find restrictions on $\{\phi_{kl}\}$. Note that it follows from Hermiticity of A, ϕ_{kk} and ϕ_{ll}, and from $\phi_{kl}^\dagger = \phi_{lk}$, that $\mathrm{Tr}[A\phi_{kk}]$, $\mathrm{Tr}[A\phi_{ll}] \in \mathbb{R}$, and that $\mathrm{Tr}[A\phi_{kl}] = (\mathrm{Tr}[A\phi_{lk}])^*$. Thus some algebra yields:

$$P_{kl} = \frac{1}{4}\begin{pmatrix} t_{kk} & ia & ib & t_{kl} \\ -ia & t_{kk} & t_{kl} & -ib \\ -ib^* & t_{kl} & t_{ll} & -ic \\ t_{kl} & ib^* & ic & t_{ll} \end{pmatrix}, \tag{10}$$
$$a = \mathrm{Tr}[A\phi_{kk}] \in \mathbb{R}, \qquad b = \mathrm{Tr}[A\phi_{kl}],$$
$$c = \mathrm{Tr}[A\phi_{ll}] \in \mathbb{R}, \qquad t_{ij} = \mathrm{Tr}[\phi_{ij}] = 1 \quad \text{or} \quad 0.$$

To proceed we require the following Lemma [17]:

Lemma 2.—If $\mathrm{Tr}[AX] = 0$ for any unitary and Hermitian matrix A then $X = 0$.

Proposition 1.—If $\phi_{kk} = 0$ or $\phi_{ll} = 0$ then $\phi_{kl} = \phi_{lk} = 0$.

Proof.—Assume that $\phi_{ll} = 0$ or $\phi_{kk} = 0$, but not both, so that either $(t_{ll} = 0,\ t_{kk} = 1)$, or $(t_{ll} = 1,\ t_{kk} = 0)$. Construct the principal submatrix obtained by deleting rows and columns 1 and 3 from P_{kl}. This leaves a principal submatrix with eigenvalues $(1 \pm \sqrt{1 + 4|b|^2})/8$. The positivity of these requires $b = \mathrm{Tr}[A\phi_{kl}] = 0$, so that by Lemma 2 $\phi_{kl} = \phi_{lk}^\dagger = 0$. When $\phi_{ll} = \phi_{kk} = 0$ the same principal submatrix has eigenvalues $\pm|b|$, so that again $\phi_{kl} = \phi_{lk}^\dagger = 0$. ■

Proposition 2.—If all of ϕ_{kk}, ϕ_{ll}, $\phi_{kl} \neq 0$ then $\phi_{kk} = \phi_{ll} = \phi_{kl} = \phi_{lk}$ [17].

It is simple to check that the only permissible case not covered by Propositions 1 and 2 is when ϕ_{kk}, $\phi_{ll} \neq 0$ and $\phi_{kl} = \phi_{lk} = 0$; in this case we have no further restrictions.

Lemma 3.—The matrix $\Phi \equiv [\phi_{ij}]$ can be decomposed as $\Phi = \bigoplus_\alpha \Phi^{(\alpha)}$, where $(\Phi^{(\alpha)})_{(i,j)\in\mathcal{D}_\Phi^{(\alpha)}} = \phi^{(\alpha)}$ (a constant) or 0.

Proof.—Every matrix is a direct sum of blocks (possibly only one). Therefore our task is to prove that the matrix elements of the αth block $\Phi^{(\alpha)}$ obey $(\Phi^{(\alpha)})_{(i,j)\in\mathcal{D}_\Phi^{(\alpha)}} = \phi^{(\alpha)}$ or 0. Collecting the results above we see that there are only four cases: Proposition $1 \Rightarrow$ (i) $\phi_{kk} = \phi_{kl} = \phi_{lk} = \phi_{ll} = 0$, (ii) $\phi_{kk} = \phi_{kl} = \phi_{lk} = 0$ and $\phi_{ll} \neq 0$; Proposition $2 \Rightarrow$ (iii) $\phi_{kk} = \phi_{kl} = \phi_{lk} = \phi_{ll} \neq 0$; (iv) ϕ_{kk}, $\phi_{ll} \neq 0$ and $\phi_{kl} = \phi_{lk} = 0$. First note that if $\phi_{kk} = 0$ then by cases (i) and (ii) also $\phi_{kl} = \phi_{lk} = 0\ \forall\ l$, i.e., the row and column crossing at a zero diagonal element must be zero. Now let $\Psi_{ij}^{(\alpha)}$ denote the 2×2 principal submatrix $\{\Phi_{ii}^{(\alpha)}, \Phi_{ij}^{(\alpha)}; \Phi_{ji}^{(\alpha)}, \Phi_{jj}^{(\alpha)}\}$, $i \neq j$. Assume $\Phi_{ij}^{(\alpha)} \neq 0$ and consider $\Psi_{ij}^{(\alpha)}$. Only case (iii) applies, so $\Phi_{ii}^{(\alpha)} = \Phi_{ij}^{(\alpha)} = \Phi_{ji}^{(\alpha)} = \Phi_{jj}^{(\alpha)}$. We can use this to show that any two block-connected diagonal elements are equal. Indeed, assume that $\Phi_{i_1i_1}^{(\alpha)}$ and $\Phi_{i_Bi_B}^{(\alpha)}$ are both nonzero and block-connected via the path $\{i_b\}_{b=2}^{B-1}$. Then by case (iii) all elements of each member of the set of principal submatrices $\{\Psi_{i_bi_{b+1}}^{(\alpha)}\}_{b=1}^{B-1}$ are equal, and since successive members always share a diagonal element, their elements are all equal, to an element we call $\phi^{(\alpha)}$. We have thus shown that $(\Phi^{(\alpha)})_{(i,j)\in\mathcal{D}_\Phi^{(\alpha)}} = \phi^{(\alpha)}$ or 0. Finally, note that case (iv) with $\phi_{kk} \neq \phi_{ll}$ can only arise between two different blocks, since if $\phi_{kk} \neq \phi_{ll}$ the previous argument shows that they cannot be block-connected. ■

We are now ready to conclude the proof of Lemma 1: It follows from Lemma 3 that $(\Phi)_{ij} = (\Phi^{(\alpha)})_{ij} = \phi^{(\alpha)}$ or 0 for $(i, j) \in \mathcal{D}_\Phi^{(\alpha)}$. Moreover, since $\rho_{SB}(0)$ is an SL class state, $\mathrm{Tr}[\phi^{(\alpha)}] = 1$. Thus the total index set $\mathcal{D}_\Phi$ for the initial state $\rho_{SB}(0)$ splits into a union of disjoint index sets $\mathcal{D}_\Phi^{(\alpha)}$, so that Eqs. (5) and (6) are satisfied, where $\rho_S(0) = \sum_\alpha\sum_{(i,j)\in\mathcal{C}_\Phi^{(\alpha)}}\varrho_{ij}|i\rangle\langle j| = \sum_\alpha\Pi_\alpha\rho_S(0)\Pi_\alpha = \sum_\alpha\sigma_S^{(\alpha)}$, where $\sigma_S^{(\alpha)} = p_\alpha\rho_S^{(\alpha)}$ and where $\rho_B^{(\alpha)} \equiv \phi^{(\alpha)}$. Here Π_α is the projector onto the subspace corresponding to block α (as defined above). Next we need to show that the ρ_B^α's are density matrices. From the properties of the $\phi^{(\alpha)}$ we already have $\mathrm{Tr}\rho_B^{(\alpha)} = 1$, so what is left to prove is that $\rho_B^{(\alpha)} > 0$. Indeed, by definition of positivity $\langle i^{(\alpha)}|\langle\psi_B|\rho_{SB}(0)|i^{(\alpha)}\rangle|\psi_B\rangle > 0$ for any state $|i^{(\alpha)}\rangle$ in the support of Π_α and any bath state $|\psi_B\rangle$. Inserting $\rho_{SB}(0) = \sum_\alpha p_\alpha\rho_S^{(\alpha)} \otimes \rho_B^{(\alpha)}$ into this inequality, we find $\langle\psi_B|\rho_B^{(\alpha)}|\psi_B\rangle > 0,\ \forall|\psi_B\rangle \in \mathcal{H}_B$. This completes the proof of necessity. Sufficiency: using the spectral decomposition $\rho_B^\alpha = \sum_j\lambda_j^\alpha|\lambda_j^\alpha\rangle\langle\lambda_j^\alpha|$ and defining $E_{ij}^\alpha \equiv \langle\beta_i|U|\lambda_j^\alpha\rangle\Pi_\alpha$: $\mathcal{H}_S \mapsto \mathcal{H}_S$, where $\{|\beta_i\rangle\}$ is an orthonormal basis for $\mathcal{H}_B$, we have, using Eqs. (1) and (5)

$$\rho_S(t) = \mathrm{Tr}_B[U\rho_{SB}(0)U^\dagger] = \sum_{\alpha ij}\lambda_i^\alpha E_{ij}^\alpha \rho_S(0) E_{ij}^{\alpha\dagger}. \qquad (11)$$

Now we simply note that if $\rho_{SB}(0)$ satisfies Eq. (6) with $\rho_B^{(\alpha)} > 0$ (i.e., $\lambda_j^\alpha > 0$), then Eq. (11) is already in the form of a CP map, with operation elements $\{\sqrt{\lambda_i^\alpha}E_{ij}^\alpha\}_{\alpha ij}$. ■

Discussion.—What is the physical meaning of fixing the bath-only operators ϕ_{ij}, as is required in our formulation? The answer is that this corresponds to fixing the initial system-bath correlations: the purely classical part is determined by the ϕ_{ii} (since $\sigma_{SB} = \sum_i \varrho_{ii}|i\rangle\langle i| \otimes \phi_{ii}$ is a VQD state with respect to the projectors $\Pi_i = |i\rangle\langle i|$), while the quantum part is determined by the ϕ_{ij} with $i \neq j$ (since $\rho_{SB} - \sigma_{SB}$ is a general non-VQD SL-state). Further, note that $\mathrm{Tr}[|j\rangle\langle i| \otimes I_B \rho_{SB}] = \varrho_{ij}\mathrm{Tr}[\phi_{ij}]$, so that non-SLness can also be written as $\mathrm{Tr}[|j\rangle\langle i| \otimes I_B\rho_{SB}] = 0$, i.e., as $\langle |i\rangle \times \langle j| \otimes I_B, \rho_{SB}\rangle = 0$ (Hilbert-Schmidt inner product $\langle A, B\rangle \equiv \mathrm{Tr}[A^\dagger B]$) and hence ρ_{SB} must lie in the hyperplane orthogonal to $|i\rangle\langle j| \otimes I_B$. Thus non-SL class states are confined to a lower-dimensional surface in the space of bipartite states, and must be *sparse*. Note that, conversely, the SL condition $\mathrm{Tr}[\phi_{ij}] = 1$ yields $\mathrm{Tr}[|j\rangle\langle i| \otimes I_B\rho_{SB}] = \varrho_{ij}$, which is not a constraint since ϱ_{ij} is arbitrary. Moreover, using a mapping from affine to linear maps [13,18], it is not hard to show that the zero-measure subset of non-SL states does not spoil Theorem 2, i.e., the QDP (1) is a linear, Hermitian map from $\rho_S(0) \mapsto \rho_S(t)$ for *any* initial state $\rho_{SB}(0)$.

Conclusions.—In this work we have identified the conditions for the validity of quantum subsystem dynamics. In particular, we have found the precise initial state conditions for the ubiquitous class of CP maps. This establishes a foundation for their widespread use in quantum information and open systems theory. We have also shown that the basic quantum-mechanical transformation (1) is always representable as a Hermitian map between the initial and final system states. This result establishes that quantum subsystem dynamics is always a meaningful concept.

Proofs.—In order to prove Theorem 2 we first need:

Lemma 4.—If $\rho_{SB}(0)$ is an SL class state then the QDP (1) is a linear map Φ_L: $\rho_S(0) \mapsto \rho_S(t)$.

Proof.—Consider the singular value decomposition (SVD) $\phi_{ij} = \sum_\alpha \lambda_\alpha^{ij}|x_{ij}^\alpha\rangle\langle y_{ij}^\alpha|$, where λ_α^{ij} are the singular values and $|x_{ij}^\alpha\rangle$ ($\langle y_{ij}^\alpha|$) are the right (left) singular vectors. Let $\{|\psi_k\rangle\}$ be an orthonormal basis for the bath Hilbert space $\mathcal{H}_B$, and define the system operators $V_{kij}^\alpha \equiv \langle\psi_k|U_{SB}|x_{ij}^\alpha\rangle$, $W_{kij}^\alpha \equiv \langle\psi_k|U_{SB}|y_{ij}^\alpha\rangle$. Since $\rho_{SB}(0)$ is an SL class state, a QDP (1) generated by an arbitrary unitary evolution U_{SB} yields (recall $\mathcal{C} \equiv \{(i,j)|\mathrm{Tr}[\phi_{ij}] = 1\}$):

$$\rho_S(t) = \mathrm{Tr}_B[\rho_{SB}(t)] = \sum_{ij}\varrho_{ij}\mathrm{Tr}_B[U_{SB}|i\rangle\langle j| \otimes \phi_{ij}U_{SB}^\dagger]$$

$$= \sum_{(i,j)\in\mathcal{C};k,\alpha}\lambda_\alpha^{ij}\varrho_{ij}V_{kij}^\alpha|i\rangle\langle j|(W_{kij}^\alpha)^\dagger. \qquad (12)$$

Now note that $P_i\rho_S(0)P_j = \varrho_{ij}|i\rangle\langle j|$, where $P_i \equiv |i\rangle\langle i|$ is a projector and $(i, j) \in \mathcal{C}$. Therefore,

$$\Phi_L[\rho_S(0)] \equiv \sum_{(i,j)\in\mathcal{C};k,\alpha}\lambda_\alpha^{ij}V_{kij}^\alpha P_i\rho_S(0)P_j(W_{kij}^\alpha)^\dagger \qquad (13)$$

$$= \sum_{(i,j)\in\mathcal{C};k,\alpha}\lambda_\alpha^{ij}\varrho_{ij}V_{kij}^\alpha|i\rangle\langle j|(W_{kij}^\alpha)^\dagger, \qquad (14)$$

which equals $\rho_S(t)$ according to Eq. (12). This defines the linear map $\Phi_L = \{E_{ijk\alpha}, E'_{ijk\alpha}\}$, whose left and right operation elements are $\{E_{ijk\alpha} \equiv \sqrt{\lambda_\alpha^{ij}}V_{kij}^\alpha P_i\}$ and $\{E'_{ijk\alpha} \equiv \sqrt{\lambda_\alpha^{ij}}W_{kij}^\alpha P_j\}$, respectively. ■

Proof of Theorem 2.—We need to show that $\rho_S(t) = \Phi_H[\rho_S(0)] = \rho_S^\dagger(t)$ if $\rho_S(0) = \rho_S^\dagger(0)$. This is now a simple calculation which uses Eqs. (13) and (14), the definitions of V_{kij}^α and W_{kij}^α, $\phi_{ij} = \phi_{ji}^\dagger$, and the SVD of ϕ_{ij}. ■

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[1] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
[2] E. C. G. Sudarshan, P. M. Mathews, and J. Rau, Phys. Rev. **121**, 920 (1961).
[3] P. Pechukas, Phys. Rev. Lett. **73**, 1060 (1994).
[4] R. Alicki, Phys. Rev. Lett. **75**, 3020 (1995).
[5] G. Lindblad, J. Phys. A **29**, 4197 (1996).
[6] P. Stelmachovic and V. Buzek, Phys. Rev. A **64**, 062106 (2001).
[7] T. F. Jordan, A. Shaji, and E. C. G. Sudarshan, Phys. Rev. A **70**, 052110 (2004).
[8] K. Życzkowski and I. Bengtsson, Open Syst. Inf. Dyn. **11**, 3 (2004).
[9] H. A. Carteret, D. R. Terno, and K. Życzkowski, Phys. Rev. A **77**, 042113 (2008).
[10] C. A. Rodríguez-Rosario *et al.*, J. Phys. A **41**, 205301 (2008).
[11] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
[12] H. Ollivier and W. H. Zurek, Phys. Rev. Lett. **88**, 017901 (2001).
[13] A. Shabani and D. A. Lidar, arXiv:0902.2478.
[14] R. D. Hill, Linear Algebra Appl. **6**, 257 (1973).
[15] M. D. Choi, Linear Algebra Appl. **10**, 285 (1975).
[16] H. Hayashi, G. Kimura, and Y. Ota, Phys. Rev. A **67**, 062109 (2003).
[17] See EPAPS Document No. E-PRLTAO-102-064912 for a proof. For more information on EPAPS, see http://www.aip.org/pubservs/epaps.html.
[18] T. F. Jordan, Phys. Rev. A **71**, 034101 (2005).

Appendix

Here, we supply the proofs of Lemma 2 and Proposition 2.

Proof of Lemma 2. Since A is unitary and Hermitian its eigenvalues are both roots of unity and real, i.e., it can always be parameterized in the form $A = UDU^\dagger$, where U is unitary and the diagonal matrix D has diagonal elements ± 1. Consider two special choices of D: $D_1 = \mathrm{diag}(+1, +1, ..., +1) = I$ and $D_2 = \mathrm{diag}(-1, +1, +1, ..., +1) = I - 2|0\rangle\langle 0|$. Since $\mathrm{Tr}[D_1 U^\dagger X U] = \mathrm{Tr}[D_2 U^\dagger X U] = 0$ we find $\mathrm{Tr}[(D_1 - D_2)U^\dagger X U] = 0$, or $\mathrm{Tr}[|0\rangle\langle 0|U^\dagger X U] = 0$. However, U is arbitrary, so that $\langle\psi|X|\psi\rangle = 0$, $\forall|\psi\rangle$ ($|\psi\rangle = U|0\rangle$). This can only be true if $X = 0$. ■

Proof of Proposition 2. After a couple of elementary row and column operations on P_{kl} we obtain:

$$P'_{kl} = \begin{pmatrix} 1_2 & B \\ B^\dagger & 1_2 \end{pmatrix}; \quad 1_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} ib & ia \\ ic & ib^* \end{pmatrix}.$$

Diagonalizing the two diagonal blocks 1_2 using $Q = \frac{1}{\sqrt{2}}(I + i\sigma_y)$ yields $P''_{kl} = Q^{\oplus 2} P'_{kl} (Q^\dagger)^{\oplus 2}$, where

$$P''_{kl} = \begin{pmatrix} C & D \\ D^\dagger & C \end{pmatrix}; \quad C = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}, \quad D = i\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix};$$

$$\alpha = (a + b + b^* + c)/2, \quad \beta = (a - b + b^* - c)/2,$$

$$\gamma = (-a - b + b^* + c)/2, \quad \delta = (-a + b + b^* - c)/2.$$

Positivity of P_{kl} implies that also $P''_{kl} > 0$, so that we can again apply the principal submatrix method. Let $e(i, j)$ denote the eigenvalues of the P''_{kl} submatrix obtained by retaining only the ith and jth rows and columns of P''_{kl}. We find $e(1, 4) = 1 \pm \sqrt{1 + |\beta|^2}$, $e(2, 3) = 1 \pm \sqrt{1 + |\gamma|^2}$ and $e(2, 4) = \pm|\alpha|^2$. Since all these eigenvalues must be positive we conclude that $\alpha = \beta = \delta = 0$, i.e., $\mathrm{Tr}[A\phi_{kk}] = \mathrm{Tr}[A\phi_{kl}] = \mathrm{Tr}[A\phi_{lk}] = \mathrm{Tr}[A\phi_{ll}]$. Applying Lemma 2 we have $\mathrm{Tr}[A(\phi_{kk} - \phi_{kl})] = 0$, so that $\phi_{kk} = \phi_{kl}$, and similarly $\phi_{kl} = \phi_{lk} = \phi_{ll}$. ■