

Ancilla models for quantum operations: For what unitaries does the ancilla state have to be physical?

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Any evolution described by a completely positive trace-preserving linear map can be imagined as arising from the interaction of the evolving system with an initially uncorrelated ancilla. The interaction is given by a joint unitary operator, acting on the system and the ancilla. Here we study the properties such a unitary operator must have in order to force the choice of a physical—that is, positive—state for the ancilla if the end result is to be a physical—that is, completely positive—evolution of the system.

I. INTRODUCTION

Consider a primary system A , with Hilbert space \mathcal{H}_A of dimension d_A , which is subjected to a superoperator \mathcal{E} , and let B be an ancillary system, with Hilbert space \mathcal{H}_B of dimension d_B . It is a commonplace that if the action of \mathcal{E} can be written as

$$\mathcal{E}(\rho_A) = \text{tr}_B(U\rho_A \otimes \sigma_B U^\dagger), \quad (1.1)$$

where U is a joint unitary operator acting on A and B and σ_B is a physical state of B (a unit-trace, positive operator, i.e., a density operator), then \mathcal{E} is a trace-preserving, completely positive (CP) map and is called a *trace-preserving quantum operation* [1, 2]. Moreover, any quantum operation can be written in the form (1.1) for some joint unitary U and some ancilla state σ_B . Quantum operations are thus the superoperator maps that can be realized physically [3]. The form (1.1) for a quantum operation is sometimes called a *Stinespring extension* [4], and we call it here an *ancilla model*.

In this paper we are interested in a different question. Suppose we know that \mathcal{E} , written as in Eq. (1.1) with U a unitary operator, is a trace-preserving quantum operation. Can we conclude that σ_B is a density operator? Generally not, as the case of a unitary transformation U_A of A makes immediately clear. Then we have $U = U_A \otimes I_B$ and $\mathcal{E}(\rho_A) = \text{tr}_B(\sigma_B)U_A\rho_A U_A^\dagger$, so σ_B can be any unit-trace operator. A natural question asks for the conditions on U such that \mathcal{E} being a trace-preserving quantum operation implies that σ_B is a density operator. Here we formulate and prove a theorem that answers this question.

In Sec. II, we spell out the problem clearly and introduce mathematical concepts that are useful in addressing the problem and proving our main result. Section III states and proves our theorem, and Sec. IV explores a number of examples that illustrate features of the main result. Section V demonstrates a curious connection to the notion of indirect state tomography, i.e., tomography on the system that can determine the state of the ancilla, and Sec. VI concludes.

II. MATHEMATICAL BACKGROUND

Before stating our theorem, we introduce some mathematical notation and concepts. Consider a system Q with Hilbert space \mathcal{H}_Q of dimension d_Q . We will consistently refer to arbitrary elements of \mathcal{H}_Q as vectors and to vectors normalized to unity as state vectors. We refer to density operators, i.e., unit-trace, positive operators, as states; pure states are rank-one density operators, i.e., one-dimensional projectors corresponding to state vectors. We sometimes use a bra-ket notation for operators on \mathcal{H}_Q , i.e., $O = |O\rangle$ and $O^\dagger = \langle O|$, and we denote the Hilbert-Schmidt operator inner product by $(N|O) = \text{tr}(N^\dagger O)$. We use a tilde to distinguish operators that are normalized to unity, i.e., $(\tilde{O}|\tilde{O}) = \text{tr}(\tilde{O}^\dagger \tilde{O}) = 1$.

A superoperator is a linear map on operators. Any superoperator \mathcal{F}_Q can be written as

$$\mathcal{F}_Q = \sum_{\alpha, \beta} \mathcal{F}_{\alpha\beta} \tilde{\tau}_\alpha \odot \tilde{\tau}_\beta^\dagger = \sum_{\alpha, \beta} \mathcal{F}_{\alpha\beta} |\tilde{\tau}_\alpha\rangle \langle \tilde{\tau}_\beta|, \quad (2.1)$$

where the operators $\tilde{\tau}_\alpha$ make up an orthonormal operator basis. The *ordinary action* of \mathcal{F}_Q on an operator O corresponds to replacing the \odot by O :

$$\mathcal{F}_Q(O) = \sum_{\alpha, \beta} \mathcal{F}_{\alpha\beta} \tilde{\tau}_\alpha O \tilde{\tau}_\beta^\dagger. \quad (2.2)$$

The *left-right action* corresponds to using the bra-ket form of \mathcal{F}_Q to operate to the left or right on operators. A superoperator \mathcal{F}_Q has a *Kraus decomposition* [5] if it can be written as

$$\mathcal{F}_Q = \sum_\alpha K_\alpha \odot K_\alpha^\dagger = \sum_\alpha |K_\alpha\rangle\langle K_\alpha|. \quad (2.3)$$

The operators K_α are called *Kraus operators*. Having a Kraus decomposition is equivalent to \mathcal{F}_Q being positive in its left-right action.

The standard way of defining complete positivity of a superoperator invokes a reference system R . A superoperator \mathcal{F}_Q is *completely positive* if $\mathcal{I}_R \otimes \mathcal{F}_Q$ maps positive operators to positive operators for all reference systems R , where $\mathcal{I}_R = I_R \odot I_R$ is the identity superoperator on R . It is clear that if \mathcal{F}_Q is left-right positive, i.e., has a Kraus decomposition, $\mathcal{I}_R \otimes \mathcal{F}_Q$ maps positive operators to positive operators, thus making \mathcal{F}_Q completely positive. Moreover, if R is chosen to have the same dimension as Q and if we introduce an (unnormalized) maximally entangled vector,

$$|\Psi\rangle = \sum_{n=1}^{d_Q} |g_n\rangle \otimes |e_n\rangle, \quad (2.4)$$

where $\{|g_n\rangle\}$ and $\{|e_n\rangle\}$ are orthonormal bases on R and Q , then we can define one-to-one, onto maps of operators on Q to vectors on RQ and of superoperators on Q to operators on RQ via

$$\begin{aligned} |O_{RQ}\rangle &\equiv I_R \otimes O_Q |\Psi\rangle &\iff \langle g_n, e_m | O_{RQ} \rangle &= \langle e_m | O_Q | e_n \rangle = (|e_m\rangle\langle e_n| | O_Q), \\ F_{RQ} &\equiv \mathcal{I}_R \otimes \mathcal{F}_Q (|\Psi\rangle\langle\Psi|) &\iff \langle g_n, e_m | F_{RQ} | g_{n'}, e_{m'} \rangle &= \langle e_m | \mathcal{F}_Q (|e_n\rangle\langle e_{n'}|) | e_{m'} \rangle = (|e_m\rangle\langle e_n| | \mathcal{F}_Q | | e_{m'}\rangle\langle e_{n'}|). \end{aligned} \quad (2.5)$$

The isomorphism between superoperators on Q and operators on RQ is called the *Choi-Jamiołkowski isomorphism* [2, 6]. The second form of Eq. (2.6) shows that the left-right positivity of \mathcal{F}_Q is equivalent to the positivity of F_{RQ} . Hence, we have the standard result that \mathcal{F}_Q is completely positive if and only if it is left-right positive.

Given any orthonormal basis of operators, $\{\tilde{\tau}_\alpha\}$, acting on \mathcal{H}_Q , we can define the unit superoperator acting in the left-right sense:

$$\mathbf{I}_Q \equiv \sum_\alpha \tilde{\tau}_\alpha \odot \tilde{\tau}_\alpha^\dagger = \sum_\alpha |\tilde{\tau}_\alpha\rangle\langle\tilde{\tau}_\alpha|. \quad (2.7)$$

By considering an outer-product basis, $\{\tilde{\tau}_{jk} = |e_j\rangle\langle e_k|\}$ for some orthonormal basis, $\{|e_j\rangle\}$, it is easy to check that

$$\mathbf{I}_Q(O) = \sum_{j,k} \tilde{\tau}_{jk} O \tilde{\tau}_{jk}^\dagger = \text{tr}(O) \mathbf{I}_Q. \quad (2.8)$$

The setting of our theorem is that U is a joint unitary operator on A and B and σ_B is an operator on B . We define a superoperator on A by its action (1.1) on density operators. We want \mathcal{E} to map density operators to density operators, so it must at least be Hermiticity- and trace-preserving. Requiring that $\mathcal{E}(\rho_A)$ be Hermitian does not imply that σ_B is Hermitian, but it does imply that $\mathcal{E}(\rho_A) = \text{tr}_B(U \rho_A \otimes \frac{1}{2}(\sigma_B + \sigma_B^\dagger) U^\dagger)$. Since the Hermitian ancilla operator $\frac{1}{2}(\sigma_B + \sigma_B^\dagger)$ gives the same map as σ_B , we can assume that σ_B is Hermitian without loss of generality. Requiring that \mathcal{E} be trace preserving implies that σ_B has unit trace.

We will need the Schmidt decomposition of U [7],

$$U = \sum_{n=1}^{R_U} A_n \otimes B_n, \quad (2.9)$$

where R_U is the Schmidt rank of U . The Schmidt operators A_n are nonzero and orthogonal,

$$(A_n | A_m) = \text{tr}_A(A_n^\dagger A_m) = (A_n | A_m) \delta_{nm}, \quad (2.10)$$

and likewise for the Schmidt operators B_n . Sometimes we want to deal with normalized operators,

$$\tilde{A}_n \equiv \frac{A_n}{\sqrt{(A_n|A_n)}} \quad \text{and} \quad \tilde{B}_n \equiv \frac{B_n}{\sqrt{(B_n|B_n)}}. \quad (2.11)$$

We can normalize either set, $\{A_n\}$ or $\{B_n\}$, by absorbing the normalization constant into the other set. That U is unitary means that

$$I = U^\dagger U = \sum_{n,m=1}^{R_U} A_n^\dagger A_m \otimes B_n^\dagger B_m, \quad (2.12)$$

which, by taking the partial trace on A , implies that

$$I_B = \frac{1}{d_A} \sum_{n=1}^{R_U} (A_n|A_n) B_n^\dagger B_n. \quad (2.13)$$

Taking the trace on B then gives

$$d_A d_B = \sum_{n=1}^{R_U} (A_n|A_n) (B_n|B_n). \quad (2.14)$$

We will need the span of the Schmidt operators B_n ,

$$\mathcal{B} \equiv \text{Span}\{ B_n \mid n = 1, 2, \dots, R_U \}, \quad (2.15)$$

and the operator orthocomplement of \mathcal{B} ,

$$\mathcal{O}_B \equiv \{ O_B \mid \text{tr}_B(B^\dagger O_B) = 0 \ \forall \ B \in \mathcal{B} \} = \{ O_B \mid \text{tr}_B(U^\dagger O_B) = 0 \}. \quad (2.16)$$

Notice that $R_U + \dim(\mathcal{O}_B) = d_B^2$.

It will also be useful to introduce a set of positive operators associated with \mathcal{B} ,

$$\mathcal{C} \equiv \{ B^\dagger B \mid B \in \mathcal{B} \}. \quad (2.17)$$

The set \mathcal{C} is not a subspace. It is a cone—i.e., any nonnegative multiple of an element of \mathcal{C} is also an element—which is a subset of the cone of positive operators on B . It is clearly a closed set. We let \mathcal{C}_1 denote the set of unit-trace elements in \mathcal{C} ; \mathcal{C}_1 is a closed and bounded subset of the closed and bounded set of density operators on B . Neither \mathcal{C} nor \mathcal{C}_1 is necessarily convex.

For the remainder of this section, we deal only with system B , so we generally omit the subscript B on vectors, operators, and superoperators. The most important set in our considerations is the set of vectors $|\phi\rangle \in \mathcal{H}_B$ such that $|\phi\rangle\langle\phi| \notin \mathcal{C}$. Any nonzero multiple of such a $|\phi\rangle$ is also in this set, but we emphasize that the set is not a subspace. For this reason, it is most convenient to represent the vectors in this set by their normalized counterparts (state vectors), so we define the following set:

$$S_B \equiv \{ \text{state vectors } |\phi\rangle \in \mathcal{H}_B \mid |\phi\rangle\langle\phi| \notin \mathcal{C} \}. \quad (2.18)$$

The set S_B is a property of the Schmidt operators B_n and, hence, a property of U .

Since we have restricted S_B to normalized vectors, we can replace the definition by

$$S_B = \{ \text{state vectors } |\phi\rangle \in \mathcal{H}_B \mid |\phi\rangle\langle\phi| \notin \mathcal{C}_1 \}. \quad (2.19)$$

We can think of S_B as the set of pure states not in \mathcal{C}_1 . Because \mathcal{C}_1 is a closed set, we can say a bit more. If the one-dimensional projector $|\phi\rangle\langle\phi|$ is not in \mathcal{C}_1 , then it lies some minimal distance away from all elements of \mathcal{C}_1 , which means that there exists a $\delta > 0$ such that $\langle\phi|C|\phi\rangle \leq 1 - \delta$ for all $C \in \mathcal{C}_1$. Slightly more generally, we can say that

$$\text{state vector } |\phi\rangle \in \mathcal{H}_B \text{ such that } |\phi\rangle\langle\phi| \notin \mathcal{C}_1 \implies \exists \ \delta > 0 \text{ such that } \langle\phi|C|\phi\rangle \leq \text{tr}(C)(1 - \delta) \ \forall \ C \in \mathcal{C}. \quad (2.20)$$

It will turn out to be useful to have available equivalent definitions of S_B . Suppose $|\psi\rangle\langle\phi| = B \in \mathcal{B}$; then $\langle\psi|\psi\rangle|\phi\rangle\langle\phi| = B^\dagger B = C$, which if $|\psi\rangle$ is not the zero vector, implies that $|\phi\rangle\langle\phi| \in \mathcal{C}$. Moreover, if $|\phi\rangle\langle\phi| = C = B^\dagger B$

for some $C \in \mathcal{C}$ (and $B \in \mathcal{B}$), the polar-decomposition theorem asserts that B is rank one, and thus $B = |\psi\rangle\langle\phi|$ for some normalized $|\psi\rangle \in \mathcal{H}_B$. Thus we have the following equivalence,

$$|\psi\rangle\langle\phi| \in \mathcal{B} \text{ for some nonzero } |\psi\rangle \in \mathcal{H}_B \iff |\phi\rangle\langle\phi| \in \mathcal{C}, \quad (2.21)$$

and its contrapositive,

$$\forall \text{ nonzero } |\psi\rangle \in \mathcal{H}_B, |\psi\rangle\langle\phi| \notin \mathcal{B} \iff |\phi\rangle\langle\phi| \notin \mathcal{C}. \quad (2.22)$$

Consider now the subspace of \mathcal{H}_B generated by the operators in the orthocomplement \mathcal{O}_B acting on a particular vector $|\phi\rangle \in \mathcal{H}_B$:

$$\mathcal{O}_B|\phi\rangle \equiv \{O|\phi\rangle \mid O \in \mathcal{O}_B\}. \quad (2.23)$$

It is easy to see that $\mathcal{O}_B|\phi\rangle$ is a subspace; it is the span of vectors $O_n|\phi\rangle$, where the set $\{O_n\}$ consists of any operators that span \mathcal{O}_B . Thus we clearly have $\dim(\mathcal{O}_B|\phi\rangle) \leq \dim(\mathcal{O}_B)$. We denote the orthocomplement of $\mathcal{O}_B|\phi\rangle$ by $(\mathcal{O}_B|\phi\rangle)^\perp$.

Because \mathcal{B} and \mathcal{O}_B are orthogonal subspaces, we have

$$|\psi\rangle\langle\phi| \in \mathcal{B} \iff \forall O \in \mathcal{O}_B, 0 = \text{tr}(O^\dagger |\psi\rangle\langle\phi|) = \langle\phi|O^\dagger|\psi\rangle \iff |\psi\rangle \in (\mathcal{O}_B|\phi\rangle)^\perp \quad (2.24)$$

and the contrapositive,

$$|\psi\rangle\langle\phi| \notin \mathcal{B} \iff |\psi\rangle \notin (\mathcal{O}_B|\phi\rangle)^\perp. \quad (2.25)$$

This gives us the following equivalence:

$$\forall \text{ nonzero } |\psi\rangle \in \mathcal{H}_B, |\psi\rangle\langle\phi| \notin \mathcal{B} \iff \mathcal{O}_B|\phi\rangle = \mathcal{H}_B. \quad (2.26)$$

Thus because of Eqs. (2.22) and (2.26), the following two ways of defining S_B are equivalent to Eqs. (2.18) and (2.19):

$$\begin{aligned} S_B &= \{ \text{state vectors } |\phi\rangle \in \mathcal{H}_B \mid \forall \text{ nonzero } |\psi\rangle \in \mathcal{H}_B, |\psi\rangle\langle\phi| \notin \mathcal{B} \} \\ &= \{ \text{state vectors } |\phi\rangle \in \mathcal{H}_B \mid \mathcal{O}_B|\phi\rangle = \mathcal{H}_B \}. \end{aligned} \quad (2.27)$$

It is useful to characterize S_B in yet another way. For this purpose, consider the orthonormal Schmidt operators, $\{\tilde{B}_n, n = 1, \dots, R_U\}$, of Eq. (2.11). Complete a basis of orthonormal operators by adding a set of orthonormal operators, $\{\tilde{O}_n \mid n = R_U + 1, \dots, d_B^2\}$, from the orthocomplement \mathcal{O}_B . We have

$$\mathbf{I} = \sum_{n=1}^{R_U} \tilde{B}_n \odot \tilde{B}_n^\dagger + \sum_{n=R_U+1}^{d_B^2} \tilde{O}_n \odot \tilde{O}_n^\dagger, \quad (2.28)$$

and for state vectors $|\phi\rangle \in \mathcal{H}_B$,

$$I = \mathbf{I}(|\phi\rangle\langle\phi|) = \sum_{n=1}^{R_U} \tilde{B}_n|\phi\rangle\langle\phi|\tilde{B}_n^\dagger + \sum_{n=R_U+1}^{d_B^2} \tilde{O}_n|\phi\rangle\langle\phi|\tilde{O}_n^\dagger. \quad (2.29)$$

A state vector $|\phi\rangle$ is in S_B if and only if the second sum on the rightmost side of Eq. (2.29) is a full-rank operator, i.e., has no zero eigenvalues. This happens if and only if the first sum on the rightmost side of Eq. (2.29) is strictly less than I ; i.e., it has largest eigenvalue strictly less than unity. Thus we can characterize S_B in the following way:

$$S_B = \left\{ \text{state vectors } |\phi\rangle \in \mathcal{H}_B \mid 1 > \left\| \sum_{n=1}^{R_U} \tilde{B}_n|\phi\rangle\langle\phi|\tilde{B}_n^\dagger \right\|_\infty \right\}. \quad (2.30)$$

Here $\|M\|_\infty$ is the operator norm that denotes the largest eigenvalue of $\sqrt{M^\dagger M}$, i.e., the largest singular value of M (for positive operators, as here, the largest eigenvalue of M).

III. MAIN THEOREM

The content of our theorem is that any rank-one projector not in \mathcal{C}_1 can be used to construct an unphysical σ_B that gives a completely positive map \mathcal{E} . Formally, we can state the theorem in the following way.

Main theorem. Let U be a joint unitary operator on A and B and σ_B be a unit-trace Hermitian operator on B . Define a Hermiticity- and trace-preserving superoperator \mathcal{E} on A by $\mathcal{E}(\rho_A) = \text{tr}_B(U\rho_A \otimes \sigma_B U^\dagger)$. \mathcal{C}_1 contains all rank-one projectors, i.e., S_B is the empty set, if and only if requiring that \mathcal{E} be a quantum operation implies that σ_B is a density operator. In symbols,

$$\begin{aligned} \forall \text{ state vector } |\phi_B\rangle \in \mathcal{H}_B, |\phi_B\rangle\langle\phi_B| \in \mathcal{C}_1 &\iff S_B = \emptyset \\ &\iff \left(\mathcal{E} \text{ a quantum operation} \implies \sigma_B \text{ is a density operator} \right). \end{aligned} \quad (3.1)$$

We use P to denote the property of U that S_B is the empty set. $\neg P$ is thus that S_B is not the empty set, i.e., that there are pure states not in \mathcal{C}_1 . Any $|\phi_B\rangle \in S_B$ can be used as an eigenstate of σ_B with negative eigenvalue in an ancilla model that gives a completely positive \mathcal{E} .

The following properties imply P and thus are sufficient to ensure that σ_B must be a density operator:

- p1. $\left(\text{tr}_B(U^\dagger O_B) = 0 \implies O_B = 0 \right)$, which is equivalent to $\dim(\mathcal{O}_B) = 0$ and $R_U = d_B^2$.
- p2. $R_U > d_B^2 - d_B$, which is equivalent to $\dim(\mathcal{O}_B) < d_B$. This property implies P because $\dim(\mathcal{O}_B|\phi_B\rangle) \leq \dim(\mathcal{O}_B)$.

The following properties imply $\neg P$ and thus are sufficient to ensure that there is a nonpositive σ_B that leads to a completely positive \mathcal{E} :

- q1. \exists a non-vanishing Hermitian operator Σ_B such that $0 = \text{tr}_B(B_n \Sigma_B B_m^\dagger) = \text{tr}_B(B_m^\dagger B_n \Sigma_B) \forall n, m$. This is equivalent to $\text{tr}_B(B \Sigma_B B^\dagger) = 0$ for all $B \in \mathcal{B}$ and thus to $\text{tr}_B(C \Sigma_B) = 0$ for all $C \in \mathcal{C}$. If a non-Hermitian operator satisfies this property, so does its conjugate, thus allowing us to construct a Hermitian operator that satisfies the property. That Σ_B is necessarily traceless follows from Eq. (2.13). Suppose we add $\mu \Sigma_B$, where μ is any real number, to a density operator σ_B that is diagonal in the same basis as Σ_B , i.e., $\sigma'_B = \sigma_B + \mu \Sigma_B$. Then σ'_B has unit trace, and the matrix G of Eq. (3.3)—and, hence, the quantum operation \mathcal{E} —remains the same, but by making $|\mu|$ large enough, we can give σ'_B negative eigenvalues. All the eigenvectors of Σ_B are elements of S_B .
- q2. $\dim(\text{Span}\{B_m^\dagger B_n \mid m, n = 1, \dots, R_U\}) < d_B^2$. This is equivalent to q1.
- q3. $R_U < d_B$, which is equivalent to $\dim(\mathcal{O}_B) \geq d_B^2 - d_B$. This property implies q2, since $\dim(\text{Span}\{B_m^\dagger B_n\}) \leq R_U^2$.

Now we are ready to give the proof.

Proof. We first reformulate the condition for complete positivity of \mathcal{E} in terms of the Schmidt operators on B . Plugging Eq. (2.9) into Eq. (1.1), we find

$$\mathcal{E} = \sum_{n,m=1}^{R_U} G_{nm} A_n \odot A_m^\dagger = \sum_{n,m=1}^{R_U} G_{nm} |A_n\rangle\langle A_m|, \quad (3.2)$$

where

$$G_{nm} \equiv (A_n | \mathcal{E} | A_m) = \text{tr}_B(B_n \sigma_B B_m^\dagger). \quad (3.3)$$

Complete positivity of \mathcal{E} is the statement that \mathcal{E} is positive in its left-right action. This is equivalent to the positivity of the matrix G , which is that $\sum_{n,m} c_n G_{nm} c_m^* \geq 0$ for all coefficients c_n , and this becomes the property

$$\text{tr}_B(B \sigma_B B^\dagger) \geq 0 \quad \forall B \in \mathcal{B}. \quad (3.4)$$

We have reduced our considerations to quantities defined on system B , so we often drop the subscript B for the rest of the proof. The complete positivity property of \mathcal{E} can now be written in the compact form

$$\text{tr}(C \sigma) \geq 0 \quad \forall C \in \mathcal{C}. \quad (3.5)$$

If P holds, \mathcal{C} contains all one-dimensional projectors, so the complete positivity condition (3.5) immediately implies that $\sigma \geq 0$. We prove the converse in the contrapositive; i.e., we show that if $\neg P$ is true, we can construct a nonpositive (unphysical) σ that is consistent with Eq. (3.5). Since P is not true, there is a state vector $|\phi\rangle$ such that $|\phi\rangle\langle\phi| \notin \mathcal{C}$ and, hence, by Eq. (2.20), a $\delta > 0$ such that $\langle\phi|C|\phi\rangle \leq \text{tr}(C)(1 - \delta)$ for all $C \in \mathcal{C}$. We lose nothing by also requiring that $\delta < 1/2$. For any such state vector, we can construct a nonpositive σ that satisfies Eq. (3.5) by letting $|\phi\rangle$ be an eigenvector with a negative eigenvalue $-\epsilon$:

$$\sigma = -\epsilon |\phi\rangle\langle\phi| + \frac{1 + \epsilon}{d_B - 1} (I - |\phi\rangle\langle\phi|), \quad \epsilon > 0. \quad (3.6)$$

For all $C \in \mathcal{C}$, we have

$$\text{tr}(C\sigma) = -\frac{1 + \epsilon d_B}{d_B - 1} \langle\phi|C|\phi\rangle + \frac{1 + \epsilon}{d_B - 1} \text{tr}(C) \geq \left(\delta \frac{1 + \epsilon d_B}{d_B - 1} - \epsilon \right) \text{tr}(C). \quad (3.7)$$

By choosing $\epsilon \leq \delta/(d_B - 1 - \delta d_B)$, we can ensure that the complete positivity condition (3.5) is satisfied for this nonpositive σ , thereby completing the proof. ■

IV. EXAMPLES

Example 1. $U = U_A \otimes U_B$. In this case, any unit-trace operator σ_B gives the same (unitary) quantum operation. There is a single Schmidt operator, U_B , on B ($R_U = 1$). The subspace \mathcal{B} is the one-dimensional subspace of all multiples of U_B , \mathcal{C} is the cone of nonnegative multiples of I_B , $\mathcal{C}_1 = \{I_B/d_B\}$, \mathcal{O}_B is the $(d_B^2 - 1)$ -dimensional space of operators of the form $U_B O$, where O is any traceless operator, and S_B contains all state vectors.

Example 2. The SWAP operator for two systems of the same Hilbert-space dimension:

$$U = \text{SWAP} = \sum_{j,k} |e_k, f_j\rangle \otimes \langle e_j, f_k| = \sum_{j,k} |e_k\rangle \langle e_j| \otimes |f_j\rangle \langle f_k|. \quad (4.1)$$

Here the vectors $|e_j\rangle$ and $|f_k\rangle$ make up any orthonormal bases for A and B . The SWAP operator acts on product states as $U\rho_A \otimes \sigma_B U^\dagger = \sigma_A \otimes \rho_B$, so it is clear that σ_B must be a density operator. Equation (4.1) is a Schmidt decomposition of SWAP. Schmidt operators on B can be taken to be the outer products $|f_j\rangle\langle f_k|$. These operators span the operator space on B , so \mathcal{B} contains all operators, \mathcal{C} is the cone of positive operators, \mathcal{C}_1 is the set of density operators, \mathcal{O}_B consists only of the zero operator, and S_B is empty.

Example 3. Two qubits with a joint unitary

$$U = e^{iX \otimes X \theta/2} = I \otimes I \cos(\theta/2) + iX \otimes X \sin(\theta/2), \quad 0 < \theta < \pi. \quad (4.2)$$

This joint unitary has Schmidt rank 2. For the unitary of Eq. (4.2), the two Schmidt operators for B can be taken to be I and X , $\mathcal{O}_B = \text{Span}\{Y, Z\}$, \mathcal{C} consists of all operators of the form $r(I + sX)$, where $r \geq 0$ and $|s| \leq 1$, \mathcal{C}_1 is the subset of \mathcal{C} with $r = 1/2$ (i.e., the density operators whose eigenstates are the eigenstates of X), and S_B contains all state vectors except the eigenstates of X .

If we write σ_B as $\sigma_B = \frac{1}{2}(I + \mathbf{s} \cdot \boldsymbol{\sigma}) = \frac{1}{2}(I + s_x X_B + s_y Y_B + s_z Z_B)$, where $\boldsymbol{\sigma}$ is the vector of Pauli operators on B , it is straightforward to show that the superoperator (1.1) on A is

$$\mathcal{E} = \cos^2(\theta/2) I \odot I + i s_x \sin(\theta/2) \cos(\theta/2) (X \odot I - I \odot X) + \sin^2(\theta/2) X \odot X = p_+ V \odot V^\dagger + p_- X V \odot V^\dagger X, \quad (4.3)$$

where $p_\pm = \frac{1}{2}(1 \pm T)$, $T = \sqrt{\cos^2 \theta + s_x^2 \sin^2 \theta}$, $V = e^{iX\alpha/2}$, and $\tan \alpha = s_x \tan \theta$. This map is a convex combination of two orthogonal unitaries, V and XV , and is completely positive if and only if $T \leq 1$, i.e., $|s_x| \leq 1$. The point here is that s_y and s_z can be anything without changing \mathcal{E} . Complete positivity only constrains s_x , in agreement with our conclusion that the only state vectors not in S_B are the eigenstates of X_B .

Any two-qubit joint unitary has Schmidt rank 1, 2, or 4 [8]. A Schmidt-rank-1 unitary is a product unitary and thus is covered by Example 1. A Schmidt-rank-2 unitary is equivalent under local unitaries to Eq. (4.2) and thus covered by Example 3. A Schmidt-rank-4 unitary has full Schmidt rank; \mathcal{C}_1 is the set of all density operators, and S_B is the empty set. Since \mathcal{C}_1 is convex in all three cases, we can conclude that for two-qubit unitaries, \mathcal{C} and \mathcal{C}_1 are always convex sets.

Example 4. A qutrit and a qubit with joint unitary

$$U = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X + |2\rangle\langle 2| \otimes Z. \quad (4.4)$$

This joint unitary has Schmidt rank 3. The Schmidt operators on B can be taken to be I , X , and Z , \mathcal{O}_B consists of all multiples of Y , \mathcal{C} is the cone of positive operators, \mathcal{C}_1 is the set of all density operators, and S_B is empty. That U satisfies p2 makes clear that S_B is empty.

For the remaining examples, we refer to an orthonormal basis, $\{|j\rangle, j = 0, \dots, d_B - 1\}$, on system B , we denote the rank-one outer products by $\tau_{jk} = |j\rangle\langle k|$, and we use the following operators on B , defined for $j < k$:

$$I_{jk} \equiv \tau_{jj} + \tau_{kk} , \quad (4.5)$$

$$Z_{jk} \equiv \tau_{jj} - \tau_{kk} , \quad (4.6)$$

$$X_{jk} \equiv \tau_{jk} + \tau_{kj} , \quad (4.7)$$

$$Y_{jk} \equiv -i(\tau_{jk} - \tau_{kj}) . \quad (4.8)$$

These are the Pauli operators for the two-dimensional subspace spanned by $|j\rangle$ and $|k\rangle$. The following operators make up a set of d_B^2 linearly independent operators, which span the space of operators on B : the unit operator I , and the operators Z_{0j} , $j = 1, \dots, d_B - 1$, span the space of diagonal operators; the operators X_{jk} , numbering $d_B(d_B - 1)/2$, and the operators Y_{jk} , numbering $d_B(d_B - 1)/2$, span the space of off-diagonal operators. These operators are pairwise orthogonal, except that $\text{tr}(Z_{0j}Z_{0k}) = 1 + \delta_{jk}$.

We can introduce an associated set of $d_B^2 - 1$ unitary operators:

$$U_j \equiv I - I_{0j} + Z_{0j} , \quad j = 1, \dots, d_B - 1, \quad (4.9)$$

$$V_{jk} \equiv I - I_{jk} + X_{jk} , \quad j < k, \quad (4.10)$$

$$W_{jk} \equiv I - I_{jk} + Y_{jk} , \quad j < k. \quad (4.11)$$

The unitary U_j is diagonal, with ones everywhere on the diagonal, except in the j th position, which has a -1 . The operators V_{jk} and W_{jk} act like the Pauli X and Y in the two-dimensional subspace spanned by $|j\rangle$ and $|k\rangle$, and act like the identity operator on the orthocomplement of this subspace. Together with the identity operator I , these operators are linearly independent and span the space of operators on B , but they are not orthogonal. To see that they span the space, one notes that the diagonal operators satisfy

$$\tau_{jj} = \frac{1}{2}(I - U_j) , \quad j = 1, \dots, d_B - 1, \quad (4.12)$$

$$\tau_{00} = \frac{1}{d_B - 1} \sum_{j=1}^{d_B-1} U_j - \frac{d_B - 3}{d_B - 1} \sum_{j=1}^{d_B-1} \tau_{jj} . \quad (4.13)$$

These expressions allow us to write any diagonal operator in terms of I and the unitaries U_j . Writing the diagonal operators $I - I_{jk}$ in terms of I and the unitaries U_j , we find that the operators X_{jk} and Y_{jk} , which span the off-diagonal subspace, can be expanded in terms of our set of unitaries.

Example 5. This example shows that P can be satisfied even though $R_U = 3d_B - 2$ is linear in d_B . The idea is to introduce a unitary U such that the set \mathcal{B} contains the operator subspace spanned by the operators τ_{0j} for $j = 0, \dots, d_B - 1$, i.e., contains all operators of the form

$$B = \lambda \sum_{j=0}^{d_B-1} b_j^* \tau_{0j} , \quad (4.14)$$

where $\lambda \geq 0$ and the expansion coefficients b_j are normalized to unity. This means that \mathcal{C} contains all operators of the form

$$B^\dagger B = \lambda^2 \sum_{j,k} b_j b_k^* \tau_{jk} = \lambda^2 |\phi\rangle\langle\phi| , \quad (4.15)$$

where

$$|\phi\rangle = \sum_j b_j |j\rangle \quad (4.16)$$

is a state vector in \mathcal{H}_B . Thus \mathcal{C}_1 contains all pure states, and $S_B = \emptyset$.

To do this, we assume that system A has dimension $3d_B - 2$, with an orthonormal basis of vectors $|0\rangle$, $|r_j\rangle$, $|s_j\rangle$, and $|t_j\rangle$, where $j = 1, \dots, d_B - 1$, and we introduce the following controlled unitary on A and B :

$$U = |0\rangle\langle 0| \otimes I + \sum_{j=1}^{d_B-1} \left(|r_j\rangle\langle r_j| \otimes U_j + |s_j\rangle\langle s_j| \otimes V_{0j} + |t_j\rangle\langle t_j| \otimes W_{0j} \right). \quad (4.17)$$

Because the projectors corresponding to the orthonormal basis on A are orthogonal and, hence, linearly independent, \mathcal{B} is the span of the target unitaries, and the operator subspace \mathcal{O}_B consists of all operators that are orthogonal to all of the target unitaries. By the same argument as above, we then have

$$\mathcal{B} = \text{Span}\{ \tau_{00}; \tau_{jj}, \tau_{0j}, \text{ and } \tau_{j0}, \text{ for } j = 1, \dots, d_B - 1 \}. \quad (4.18)$$

As noted above, in this situation, \mathcal{C}_1 contains all pure states and thus P is satisfied.

We can go a bit further and characterize the entire set \mathcal{C}_1 . An arbitrary element of \mathcal{B} has the form

$$B = \lambda \sum_{j=0}^{d_B-1} b_j^* \tau_{0j} + \sum_{j=1}^{d_B-1} \mu_j (c_j^* \tau_{j0} + d_j^* \tau_{jj}), \quad (4.19)$$

where λ and μ_j are real and nonnegative, the expansion coefficients b_j are normalized to unity, and $|c_j|^2 + |d_j|^2 = 1$. The general element of \mathcal{C} looks like

$$C = \lambda^2 |\phi\rangle\langle\phi| + \sum_{j=1}^{d_B-1} \mu_j^2 (c_j |0\rangle + d_j |j\rangle) (c_j^* \langle 0| + d_j^* \langle j|), \quad (4.20)$$

where $|\phi\rangle$ is the state vector of Eq. (4.16). Thus the general element of \mathcal{C}_1 is a convex combination of an arbitrary pure state $|\phi\rangle\langle\phi|$ and the pure states in the sum in Eq. (4.20).

We can use this example to show that \mathcal{C}_1 (and \mathcal{C}) are not generally convex sets. If \mathcal{C}_1 were a convex set, then since it contains all pure states, it would have to contain all density operators, but it is easy to find density operators not in \mathcal{C}_1 for $d_B \geq 4$. For this purpose, we restrict attention to operators that are orthogonal to $|0\rangle$. The general form of an element of \mathcal{C}_1 of this sort is

$$C = \lambda^2 \sum_{j,k=1}^{d_B} b_j b_k^* |j\rangle\langle k| + \sum_{j=1}^{d_B} \mu_j^2 |j\rangle\langle j|. \quad (4.21)$$

Let Π be the projector onto the subspace orthogonal to $|0\rangle$, and let Σ be any traceless, Hermitian operator that is orthogonal to $|0\rangle$, scaled so that its most negative eigenvalue is -1 . Then $\sigma = (\Pi + \epsilon\Sigma)/(d_B - 1)$ is a density operator for $0 \leq \epsilon \leq 1$; when $\epsilon = 1$, σ is on the boundary of the space of density operators. For this density operator to be in \mathcal{C}_1 , we must have $\lambda^2 b_j b_k^* = \epsilon \Sigma_{jk}/(d_B - 1)$. When $d_B \geq 4$, we can let $\Sigma_{12} = \Sigma_{23} = -\Sigma_{13}$ be real and positive; then there is no way to choose the phases of b_1 , b_2 , and b_3 to satisfy the condition if $\epsilon \neq 0$, thus showing that σ is not in \mathcal{C}_1 for $0 < \epsilon \leq 1$.

It is worth spelling this out in three dimensions ($d_B = 3$), where the target unitaries on B have the following matrix representations:

$$\begin{aligned} I &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & U_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & U_2 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\ V_{01} &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & V_{02} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & W_{01} &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & W_{02} &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 0 \end{pmatrix}. \end{aligned} \quad (4.22)$$

We can see explicitly in this case that \mathcal{B} has the form given in Eq. (4.18). The orthocomplement \mathcal{O}_B , being orthogonal to all the target unitaries, is

$$\mathcal{O}_B = \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \right\} = \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \right\}. \quad (4.23)$$

Any operator $O_B \in \mathcal{O}_B$ has all zeros in the its first row, so $\langle 0|O_B|\phi\rangle = 0$ for any vector $|\phi\rangle$, implying that $S_B = \emptyset$. This way of showing that S_B is the empty set, by showing that all elements of \mathcal{O}_B have all zeroes in the first row, works for any value of d_B .

Example 6. It is easy now to formulate an example where P holds and $R_U = 2d_B$. To do so, we consider the controlled unitary

$$U = |0\rangle\langle 0| \otimes I + |r_1\rangle\langle r_1| \otimes U'_1 + \sum_{j=1}^{d_B-1} \left(|s_j\rangle\langle s_j| \otimes V_{0j} + |t_j\rangle\langle t_j| \otimes W'_{0j} \right). \quad (4.24)$$

where the unitaries on B are defined by

$$U'_1 = I - I_{01} - Z_{01}, \quad (4.25)$$

$$V_{0j} = I - I_{0j} + X_{0j}, \quad (4.26)$$

$$W'_{0j} \equiv I - I_{0j} - iY_{0j}. \quad (4.27)$$

It is easy to convince oneself that the target unitaries are linearly independent and thus that $R_U = 2d_B$. Moreover, since $\tau_{00} = (I - U'_1)/2$ and $\tau_{0j} = (V_{0j} - W'_{0j})/2 = (X_{0j} + iY_{0j})/2$ for $j = 1, \dots, d_B - 1$, we are in the situation discussed in Example 5, so $S_B = \emptyset$.

Example 7. In this example, we demonstrate that $\neg P$ is possible when $R_U = d_B^2 - d_B$, thus showing that condition p2 is optimal. We assume that system A has dimension $d_B^2 - d_B$, and we use the controlled unitary

$$U = |0\rangle\langle 0| \otimes I + \sum_{j=1}^{d_B-1} |r_j\rangle\langle r_j| \otimes U_j + \sum_{j=1}^{d_B-1} \sum_{k=j+1}^{d_B-1} \left(|s_{jk}\rangle\langle s_{jk}| \otimes V_{jk} + |t_{jk}\rangle\langle t_{jk}| \otimes W_{jk} \right) + \sum_{j=2}^{d_B-1} |t_{0j}\rangle\langle t_{0j}| \otimes W_{0j}, \quad (4.28)$$

where the indicated vectors on A make up an orthonormal basis. As in Example 5, \mathcal{B} is the span of the target unitaries and thus can be written as

$$\mathcal{B} = \text{Span}\{ \tau_{00}; \tau_{jk}, \text{ for } j, k = 1, \dots, d_B - 1; Y_{0j}, \text{ for } j = 2, \dots, d_B - 1 \}, \quad (4.29)$$

and the orthocomplement of \mathcal{B} is

$$\mathcal{O}_B = \text{Span}\{ \tau_{01}, \tau_{10}; X_{0j}, \text{ for } j = 2, \dots, d_B - 1 \}. \quad (4.30)$$

Letting $|\phi\rangle = |0\rangle + |1\rangle$, we clearly have $\mathcal{O}_B|\phi\rangle = \mathcal{H}_B$ and thus $\neg P$. Indeed, it is easy to see that the state vectors not in S_B are those that are orthogonal to $|0\rangle$ or to $|1\rangle$.

To introduce our last example, we consider the Weyl (or generalized Pauli) unitary operators

$$B_{kl} = X^k Z^l, \quad k, l = 0, \dots, d_B - 1, \quad (4.31)$$

where X and Z are the shift and phase operators in the standard basis, i.e., $X|j\rangle = |(j+1) \bmod d_B\rangle$ and $Z|j\rangle = e^{i2\pi j/d_B}|j\rangle$. The Weyl operators (4.31) are pairwise orthogonal. The eigenstates of X are the Fourier-transformed basis states

$$|\overline{k}\rangle = \frac{1}{\sqrt{d_B}} \sum_{j=0}^{d_B-1} e^{i2\pi jk/d_B} |j\rangle. \quad (4.32)$$

We have $X|\overline{k}\rangle = e^{-i2\pi k/d_B}|\overline{k}\rangle$ and $Z|\overline{k}\rangle = |(k+1) \bmod d_B\rangle$.

We assume the existence of a fiducial state vector $|\phi\rangle$ such that the state vectors $|\phi_{kl}\rangle = B_{kl}|\phi\rangle$ form a SIC-POVM, i.e.,

$$|\langle \phi_{kl} | \phi_{k'l'} \rangle|^2 = \frac{1}{d_B + 1} \quad \text{when } kl \neq k'l'. \quad (4.33)$$

The existence of such a fiducial vector for all d_B was conjectured by Zauner [9]; the conjecture has been demonstrated for $d_B = 1, \dots, 15, 19, 24, 35$, and 48 and numerically up to at least $d_B = 67$ (see [10] and references therein). Notice that any vector in the SIC-POVM could be used as the fiducial vector.

Consider now the class of controlled unitaries with Schmidt decomposition

$$U = \sum_{n=1}^{R_U} |n\rangle\langle n| \otimes B_n, \quad (4.34)$$

where the operators B_n , indexed by the single index n , comprise a subset of R_U elements drawn from the Weyl operators (4.31). The form (4.34) is a Schmidt decomposition of U , and the Weyl operators B_n are Schmidt operators on system B .

According to (2.30), the fiducial state vector $|\phi\rangle$ is in S_B if and only if

$$\left\| \sum_{n=1}^{R_U} B_n |\phi\rangle\langle\phi| B_n^\dagger \right\|_\infty = \left\| \sum_{n=1}^{R_U} |\phi_n\rangle\langle\phi_n| \right\|_\infty = \|\Phi\|_\infty < d_B. \quad (4.35)$$

Here we define

$$\Phi \equiv \sum_{n=1}^{R_U} |\phi_n\rangle\langle\phi_n| \quad (4.36)$$

to be the sum of the projectors onto the subset of SIC-POVM vectors. Our task is to bound the operator norm of Φ in terms of R_U .

To do so, we consider a purification of Φ into an R_U -dimensional system S :

$$|\Phi_{SB}\rangle \equiv \sum_{n=1}^{R_U} |n\rangle \otimes |\phi_n\rangle. \quad (4.37)$$

Since $|\Phi_{SB}\rangle$ is rank one, the spectrum of Φ is the same as the spectrum of the reduced matrix of $|\Phi_{SB}\rangle\langle\Phi_{SB}|$ on S , which is the Gram matrix of the vectors $|\phi_n\rangle$:

$$\text{tr}_B(|\Phi_{SB}\rangle\langle\Phi_{SB}|) = \sum_{n,m=1}^{R_U} \langle\phi_m|\phi_n\rangle |n\rangle\langle m|. \quad (4.38)$$

Applying the condition (4.33) that the vectors $|\phi_n\rangle$ form a SIC POVM gives

$$\text{tr}_B(|\Phi_{SB}\rangle\langle\Phi_{SB}|) = \sum_{n=1}^{R_U} |n\rangle\langle n| + \frac{1}{\sqrt{d_B+1}} \sum_{\substack{n,m=1,\dots,R_U \\ n \neq m}} e^{i\theta_{nm}} |n\rangle\langle m| \quad (4.39)$$

$$= \left(1 - \frac{1}{\sqrt{d_B+1}}\right) I_S + \frac{1}{\sqrt{d_B+1}} \sum_{n,m=1}^{R_U} e^{i\theta_{nm}} |n\rangle\langle m|, \quad (4.40)$$

with $\theta_{nm} = \arg(\langle\phi_n|\phi_m\rangle) = -\theta_{mn}$. Since the first term in Eq. (4.40) is proportional to the identity on S , we only need to bound the norm of the second term, which we do by considering an arbitrary normalized vector $|c\rangle = \sum_{n=1}^{R_U} c_n |n\rangle$:

$$\left\langle c \left| \left(\sum_{n,m=1}^{R_U} e^{i\theta_{nm}} |n\rangle\langle m| \right) \right| c \right\rangle = \sum_{n,m=1}^{R_U} e^{i\theta_{nm}} c_n^* c_m \leq \sum_{n,m=1}^{R_U} |c_n| |c_m| = \left(\sum_{n=1}^{R_U} |c_n| \right)^2 \leq R_U. \quad (4.41)$$

Putting everything together, we obtain

$$\|\Phi\|_\infty = \left\| \text{tr}_B(|\Phi_{SB}\rangle\langle\Phi_{SB}|) \right\|_\infty \leq 1 + \frac{R_U - 1}{\sqrt{d_B+1}}. \quad (4.42)$$

The right-hand-side of Eq. (4.42) is strictly smaller than d_B whenever

$$R_U \leq \lceil \sqrt{d_B+1}(d_B-1) \rceil. \quad (4.43)$$

Here $\lceil x \rceil$ denotes the smallest integer larger than or equal to x .

We conclude from the condition (4.35) that $S_B \neq \emptyset$ for $R_U \leq \lceil \sqrt{d_B + 1}(d_B - 1) \rceil$, regardless of the specific choice of the R_U Weyl operators B_n in Eq. (4.34). In particular, S_B contains the fiducial vector $|\phi\rangle$. We now examine in detail a particular case of the joint unitary (4.34).

Example 8. Consider the controlled unitary (4.34) with the specific choice of $R_U = 2d_B - 1$ Weyl operators

$$\{I, Z, \dots, Z^{d_B-1}, X, \dots, X^{d_B-1}\}. \quad (4.44)$$

For $d_B \geq 4$, condition (4.43) is satisfied; hence the fiducial state vector is contained in S_B . Moreover, the special Fourier structure of this case makes it easy to determine all the elements of the set S_B for $d_B \geq 3$ (the case $d_B = 2$ is equivalent to our Example 4). To do this, we find the set of state vectors contained in \mathcal{C}_1 ; S_B is the complementary set. For $d_B \geq 3$, we now show that the state vectors in \mathcal{C}_1 are the eigenstates $|\bar{j}\rangle$ of X and the eigenstates $|j\rangle$ of Z .

The general element of \mathcal{B} ,

$$B = \lambda I + \sum_{j=1}^{d_B-1} (\eta_j X^j + \zeta_j Z^j), \quad (4.45)$$

has the matrix representation in the standard basis,

$$B = \begin{pmatrix} \bar{\zeta}_0 & \eta_{d_B-1} & \eta_{d_B-2} & \cdots & \eta_1 \\ \eta_1 & \bar{\zeta}_1 & \eta_{d_B-1} & \cdots & \eta_2 \\ \eta_2 & \eta_1 & \bar{\zeta}_2 & \cdots & \eta_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \eta_{d_B-1} & \eta_{d_B-2} & \eta_{d_B-3} & \cdots & \bar{\zeta}_{d_B-1} \end{pmatrix}, \quad (4.46)$$

where

$$\bar{\zeta}_j = \lambda + \sum_{k=1}^{d_B-1} e^{i2\pi jk/d_B} \zeta_k. \quad (4.47)$$

The matrix B is rank one if and only if all the order-two minors (determinants of 2×2 submatrices) are zero.

We first note that minor condition implies that if any of the η_j s is nonzero, then all the matrix elements of B —hence, all the η_j s—are nonzero. We deal with this case first. The condition on minors can then be restated as the requirement that the ratio of matrix elements in the same row of different columns is independent of row, and these reduce to the following conditions:

$$\frac{\eta_1}{\bar{\zeta}_{j+1}} = \frac{\eta_2}{\eta_1} = \frac{\eta_3}{\eta_2} = \cdots = \frac{\eta_{d_B-1}}{\eta_{d_B-2}} = \frac{\bar{\zeta}_j}{\eta_{d_B-1}}, \quad j = 0, \dots, d_B - 1. \quad (4.48)$$

For $d_B = 2$, this is a single condition, $\eta_1^2 = \bar{\zeta}_0 \bar{\zeta}_1 = \lambda^2 - \zeta_1^2$; as mentioned above, this takes us back to Example 4, where $S_B = \emptyset$. For $d_B \geq 3$, we have immediately that all the $\bar{\zeta}_j$ s are equal and thus that $\zeta_j = 0$ for $j = 1, \dots, d_B - 1$ and $\bar{\zeta}_j = \lambda$ for $j = 0, \dots, d_B - 1$. Now we can find the solutions of conditions (4.48), labeled by $k = 0, \dots, d_B - 1$:

$$\eta_j = \lambda e^{i2\pi jk/d_B}. \quad (4.49)$$

This gives $B_k = d_B \lambda |\bar{k}\rangle \langle k|$. We now turn to the case where all of the η_j s are zero. In this situation, the minor condition immediately tells us that only one diagonal element of B can be nonzero. We can also deal efficiently with this case by moving to the Fourier basis, which switches the roles of X and Z and of the η_j s and ζ_j s; then one similarly concludes that all the η_j s are zero and that $\zeta_j = \lambda e^{-i2\pi jk/d_B}$ and $\bar{\zeta}_j = d_B \lambda \delta_{jk}$, $k = 0, \dots, d_B - 1$, giving $B_k = d_B \lambda |k\rangle \langle k|$. This shows that the pure states in \mathcal{C}_1 are the eigenstates of X and Z . All other state vectors are in S_B .

V. INDIRECT TOMOGRAPHY

Suppose that S_B is not the empty set so that, as we have learned, there are unphysical ancilla “states” $\sigma_B \not\geq 0$ such that the map (1.1) is a proper quantum operation. One can ask whether this happens because the unphysicality

of the ancilla is “hidden” and irrelevant. In the example given in the Introduction, i.e., a joint unitary $U = U_A \otimes I_B$, the ancilla does not interact with the system; the evolution the system undergoes is independent of the “state” of the ancilla. We will now show that this is not always the case: a counterintuitive situation can arise, where (i) the joint unitary U can lead to an operation on the system even in cases where the “state” of the ancilla is unphysical, i.e., $S_B \neq \emptyset$, yet (ii) at the same time, U allows the tomographic reconstruction of the “state” of the ancilla.

By this we mean the following. Recall Eqs. (1.1), (3.2), and (3.3),

$$\mathcal{E}_\sigma(\rho_A) \equiv \text{tr}_B(U\rho_A \otimes \sigma_B U^\dagger) = \sum_{n,m=1}^{R_U} G_{nm} A_n \rho_A A_m^\dagger, \quad (5.1)$$

where $G_{nm} \equiv (A_n | \mathcal{E}_\sigma | A_m) = \text{tr}_B(B_n \sigma_B B_m^\dagger)$, and the operators A_n and B_n are Schmidt operators for U , as in Eq. (2.9). We can use standard process tomography to determine \mathcal{E}_σ from measurements of an informationally complete POVM on the output states obtained from an informationally complete set of input states. We say that U allows *indirect tomography* on B if this knowledge of \mathcal{E}_σ uniquely determines σ_B . This is equivalent to saying that the matrix G_{nm} determines σ_B .

To allow such indirect tomography on the ancilla state, all we need is that different operators σ_B map to different matrices G_{nm} . This map being linear, we require that $\text{tr}_B(B_n O_B B_m^\dagger) = 0$, for $n, m = 1, \dots, R_U$, implies $O_B = 0$ or, equivalently, that the operators $B_m^\dagger B_n$ span the space of operators on \mathcal{H}_B . Thus we reach our theorem on indirect tomography.

Theorem. Indirect tomography. The unitary U with Schmidt decomposition $U = \sum_{n=1}^{R_U} A_n \otimes B_n$ allows indirect tomography if and only if

$$\dim(\text{Span}\{B_m^\dagger B_n \mid m, n = 1, \dots, R_U\}) = d_B^2. \quad (5.2)$$

We want to exhibit unitaries that allow indirect tomography even if $S_B \neq \emptyset$. We do not have to go far: Examples 7 and 8 of Sec. IV have exactly this property. In Example 8, it is not hard to see that the set $\{B_m^\dagger B_n \mid m, n = 1, \dots, 2d_B - 1\}$ comprises *all* Weyl operators (up to irrelevant phases), which means that the unitary (4.34) allows indirect tomography.

By definition, when an interaction unitary U allows indirect tomography there is only *one* “state” σ_B of the ancilla compatible with the evolution \mathcal{E}_σ . Thus the situation incarnated by Examples 7 and 8 clarifies that the complete positivity of the evolution \mathcal{E}_σ undergone by A , in spite of the lack of physicality of σ_B , cannot be interpreted as saying that there is some other *physical* state $\sigma'_B \geq 0$ of the ancilla such that $\mathcal{E}_\sigma = \mathcal{E}_{\sigma'}$.

VI. CONCLUSION

We have introduced, answered, and explored the question of what properties a joint unitary operator, acting on a system and an ancilla, must have in order that a quantum operation on the system, based on this joint unitary, requires that the ancilla state be physical. The answer uncovers structures, not hitherto appreciated, on the space of states of the ancilla, structures clearly connected to the question of when a superoperator is a completely positive.

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