A Schmidt number for density matrices

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We introduce the notion of a Schmidt number of a bipartite density matrix, characterizing the minimum Schmidt rank of the pure states that are needed to construct the density matrix. We prove that Schmidt number is nonincreasing under local quantum operations and classical communication. We show that k-positive maps witness Schmidt number, in the same way that positive maps witness entanglement. We show that the family of states which is made from mixing the completely mixed state and a maximally entangled state have increasing Schmidt number depending on the amount of maximally entangled state that is mixed in. We show that Schmidt number *does not necessarily increase* when taking tensor copies of a density matrix ρ; we give an example of a density matrix for which the Schmidt numbers of ρ and $\rho \otimes \rho$ are both 2.

In quantum information theory the study of bipartite entanglement is of great importance. The usual scenario is one in which two parties, Alice and Bob, share a supply of n pure or mixed states $\rho^{\otimes n}$ which they would like to convert by Local Operations and Classical Communication (denoted as $LO + CC$) to a supply of k other mixed or pure states $\sigma^{\otimes k}$, where k can either be smaller or larger than n. The simple question that underlies many studies in bipartite entanglement is the question: what properties of these two sets of states make it possible or impossible to carry out such a protocol? Much work has been devoted to developing the necessary and sufficient conditions for this $LO + CC$ convertability. In the case of pure state convertability, it has been found that some aspects of this problem can be understood with the mathematics of majorization [1]. In the case of mixed state entanglement the theory of positive maps has been shown to play an important role [2]. The power of positive maps is best illustrated by the Peres separability condition [3] which says that a bipartite density matrix which is unentangled (aka separable) must be positive under the application of the partial transposition map. For low dimensional spin systems this condition is not only necessary but also sufficient to ensure separability [2]. It has been shown [4] that density matrices which are positive under partial transposition are undistillable, that is, nonconvertible by $LO + CC$ to sets of entangled pure states. Many examples of these bound entangled states have been found [5–8]. Evidence has been found as well for the nondistillability of certain classes of entangled states which are not positive under partial transposition [9,10], and it was shown that this feature relates to the 2-positivity of certain maps [9].

In this paper, we extend the $LO + CC$ classification of bipartite mixed states with the use of positive maps. In particular, we extend the notion of the Schmidt rank of a pure bipartite state to the domain of bipartite density matrices. We will show that this new quantity, which we will call *Schmidt number*, is witnessed by k-positive maps.

For a bipartite pure state which we write in its Schmidt decomposition (see Ref. [11])

$$|\psi\rangle = \sum_{i=1}^{k} \sqrt{\lambda_i}|a_i\rangle \otimes |b_i\rangle, \tag{1}$$

the number k is the Schmidt rank of the pure state; it is the rank of the reduced density matrix $\rho_{red} = \mathrm{Tr}_B|\psi\rangle\langle\psi|$. A necessary condition for a pure state to be convertible by $LO + CC$ to another pure state, is that the Schmidt rank of the first pure state is larger than or equal to the Schmidt rank of the latter pure state; local operations and classical communication cannot increase the Schmidt rank of a state [12]. When we extend this number to the domain of mixed states, we will require that this property of no increase of Schmidt number by $LO + CC$ still holds. We propose the following definition which is a natural extension of the one applied to pure states.

Definition 1 *A bipartite density matrix ρ has Schmidt number k if (i) for any decomposition of ρ, $\{p_i \geq 0, |\psi_i\rangle\}$ with $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ at least one of vectors $\{|\psi_i\rangle\}$ has at least Schmidt rank k and (ii) there exists a decomposition of ρ with all vectors $\{|\psi_i\rangle\}$ of Schmidt rank at most k.*

The Schmidt number of a pure state $|\psi\rangle$ is simply the Schmidt rank of the pure state. The Schmidt number of a separable state is 1. Let us denote the set of density matrices on $\mathcal{H}_n \otimes \mathcal{H}_n$ that have Schmidt number k or less by S_k. The set S_k is a convex compact subset of the entire set of density matrices denoted by S, and $S_{k-1} \subset S_k$. The set of separable density matrices is S_1.

The set S_1 has been completely characterized by positive maps [2]. Namely, for any state ρ defined on $\mathcal{H}_n \otimes \mathcal{H}_n$, $\rho \in S_1$ holds if and only if the matrix $(\mathbf{1} \otimes \Lambda_1)(\rho)$ has non-negative eigenvalues for all positive maps $\Lambda_1 : \mathcal{M}_n(\mathcal{C}) \to \mathcal{M}_n(\mathcal{C})$ [13].

Now let us recall the definition of k-positive linear maps:

Definition 2 *The linear Hermiticity-preserving map Λ is k-positive if and only if*

$$(\mathbf{1} \otimes \Lambda)(|\psi\rangle\langle\psi|) \geq 0, \tag{2}$$

for all $|\psi\rangle\langle\psi| \in S_k$.

It is not hard to show that when a positive map $\Lambda_n : \mathcal{M}_n(\mathcal{C}) \to \mathcal{M}_m(\mathcal{C})$ is n-positive, Λ_n is completely positive [14]. Similarly as with the characterization of S_1 in terms of 1-positive (or, equivalently, positive) maps, we can characterize S_k with k-positive maps:

Theorem 1 *Let ρ be a density matrix on $\mathcal{H}_n \otimes \mathcal{H}_n$. The density matrix ρ has Schmidt number at least $k+1$ if and only if there exists a k-positive linear map Λ_k such that*

$$(\mathbf{1} \otimes \Lambda_k)(\rho) \not\geq 0. \tag{3}$$

The proof of this theorem, which involves some technical details, is given at the end of this paper. With our definition of Schmidt number, it is not hard to prove that

Proposition 1 *The Schmidt number of a density matrix cannot increase under local quantum operations and classical communication.*

Proof Consider a density matrix ϱ which has some Schmidt number k. Then it has the form $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ with all vectors $|\psi_i\rangle$ having Schmidt rank at most k. If there were any $LO + CC$ operation which would increase the Schmidt number of the state, it would increase the Schmidt rank of least one of the pure states $|\psi_i\rangle\langle\psi_i|$. But no $LO + CC$ operation can increase the Schmidt rank of a pure state [12]. $\square$

We will study a well known class of states ρ_F, mixtures of the completely mixed state and a maximally entangled state, by which we illustrate the notion of Schmidt number and its relation to k-positive maps. First we note the following:

Lemma 1 *For any density matrix ρ on $\mathcal{H}_N \otimes \mathcal{H}_N$ that has Schmidt number k, we have*

$$f(\rho) \equiv \max_{\Psi} \langle\Psi| \rho |\Psi\rangle \leq \frac{k}{N}, \tag{4}$$

where we maximize over maximally entangled states $|\Psi\rangle$.

Proof For any pure state $|\psi\rangle\langle\psi|$ with Schmidt rank k characterized by its Schmidt coefficients $\{\lambda_i\}$, see Eq. (1), the function f equals [15]

$$f(|\psi\rangle\langle\psi|) = \frac{1}{N} \left[\sum_{i=1}^{N} \sqrt{\lambda_i} \right]^2. \tag{5}$$

Using Lagrange multipliers to implement the constraint $\sum_i \lambda_i = 1$ one can show that $[\sum_{i=1}^{N} \sqrt{\lambda_i}]^2 \leq k$. Since ρ has Schmidt number k, $f(\rho) = \max_{\Psi} \sum_i p_i \langle\Psi|\psi_i\rangle\langle\psi_i|\Psi\rangle \leq \frac{k}{N}$. $\square$

We consider the family of states

$$\rho_F = \frac{1-F}{N^2-1} \left(\mathbf{1} - |\Psi^+\rangle\langle\Psi^+| \right) + F|\Psi^+\rangle\langle\Psi^+|,$$
$$0 \leq F \leq 1, \tag{6}$$

with $|\Psi^+\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} |ii\rangle$. When $F \leq \frac{1}{N}$ the density matrix ρ_F is separable while for $F > \frac{1}{N}$ it can be distilled by an explicit protocol (see Ref. [15]).

For these states we have $f(\rho_F) = F$. Therefore by Lemma 1, when $F > \frac{k}{N}$ the state has Schmidt number at least $k+1$. This result has an alternative derivation in terms of k-positive maps. There exists a well known family of k-positive maps for which the following has been proved:

Lemma 2 *[16,17] Let Λ_p be a family of positive maps on $\mathcal{M}_N(\mathcal{C})$ of the form*

$$\Lambda_p(X) = \mathrm{Tr}\, X \mathbf{1} - pX, \tag{7}$$

where $X \in \mathcal{M}_N$. The map Λ_p is k-positive, but $k+1$-negative ($k < N$) for

$$\frac{1}{k+1} < p \leq \frac{1}{k}. \tag{8}$$

Note that the range of p for k-positivity does not depend on the dimension N of $\mathcal{H}_N$. We note that the map $\Lambda_{p=1}$ is the reduction criterion that was used in Ref. [15] to develop a distillation method for entangled density matrices on $\mathcal{H}_N \otimes \mathcal{H}_N$. If we apply these maps Λ_p on half of ρ_F, we find the same lower bound on the Schmidt number of ρ_F.

By giving an explicit decomposition of ρ_F, we will show that this lower bound on the Schmidt number is tight. We will do so by showing that the density matrix ρ_F at the point $F = \frac{k}{N}$ can be made by mixing Schmidt rank k vectors. If we show that at $F = \frac{k}{N}$ the density matrix can be made by mixing Schmidt rank k vectors, then it follows that at any $F < \frac{k}{N}$ only vectors with Schmidt rank k are needed, as we can make these states by mixing the completely mixed state $\mathbf{1}$ with the density matrix $\rho_{F=k/N}$. As observed in Ref. [15], the states ρ_F have

the important property that they are invariant under the operation $U \otimes U^*$ for any unitary transformation U. We can define the $LO + CC$ superoperator $\mathcal{S}^{U \otimes U^*}$ as

$$\mathcal{S}^{U \otimes U^*}(\rho) = \frac{1}{Vol(U)} \int dU \, U \otimes U^* \rho \, U^\dagger \otimes U^{*\dagger}, \quad (9)$$

which will bring any initial state ρ into the form of ρ_F, i.e. a mixture of $\mathbf{1}$ and $|\Psi^+\rangle\langle\Psi^+|$.

As our initial state we take the maximally entangled Schmidt rank k state

$$|\psi_k\rangle = \frac{1}{\sqrt{k}} \sum_{i=1}^{k} |ii\rangle, \quad (10)$$

and let $\mathcal{S}^{U \otimes U^*}$ operate on this state. We easily find that the resulting density matrix equals $\frac{k}{N}|\Psi^+\rangle\langle\Psi^+| + \frac{1-k/N}{N^2-1}(\mathbf{1} - |\Psi^+\rangle\langle\Psi^+|)$ which is the desired result. We can summarize these results in a theorem:

Theorem 2 *The state ρ_F in $\mathcal{H}_N \otimes \mathcal{H}_N$ has Schmidt number k if and only if*

$$\frac{k-1}{N} < F \leq \frac{k}{N}. \quad (11)$$

For this special class of states we have found that Schmidt number is monotonically related to the amount of entanglement in the state. This is not always the case; a pure state $|\psi\rangle$ with Schmidt rank k can have much less entanglement than, say, the 1 bit of a maximally entangled Schmidt rank 2 state.

When we find that a density matrix ρ is of Schmidt number k, we may ask whether the tensor product $\rho \otimes \rho$ is of Schmidt number k^2. Or is it possible to make $\rho \otimes \rho$ from Schmidt rank $m < k^2$ vectors? In other words, when we assign the value $\mathcal{N}(\rho) = \log k$ to a density matrix ρ which has Schmidt number k, we ask whether $\mathcal{N}(\rho)$ is *additive*, i.e.

$$\mathcal{N}(\rho^{\otimes n}) = n \log k. \quad (12)$$

For pure states this additivity property holds: The tensor product of two pure entangled states, each with Schmidt rank k, is a pure state with Schmidt rank k^2. With a simple argument we can lower bound the function $\mathcal{N}(\rho)$. When ρ itself has Schmidt number k, then the Schmidt number of any number of copies of ρ, $\rho^{\otimes n}$, must be at least k. We can get ρ from $\rho^{\otimes n}$ ($n \geq 2$) by local operations, namely tracing out all states but one. Therefore $\rho^{\otimes n}$ cannot have a smaller Schmidt number than ρ itself, since, if it were, then we find a contradiction with Proposition 1. Thus we obtain the bound

$$\mathcal{N}(\rho^{\otimes n}) \geq \mathcal{N}(\rho). \quad (13)$$

Let us consider tensor copies of the state ρ_F, i.e. $\rho_F^{\otimes m}$ with $m \geq 2$ and lower bound the Schmidt number as

before. This time, in the space $\mathcal{H}_{N^m} \otimes \mathcal{H}_{N^m}$ we have $f(\rho_F^{\otimes m}) \geq F^m$ and with Lemma 1 this implies that when $F^m > \frac{k}{N^m}$ the Schmidt number of $\rho_F^{\otimes m}$ is at least $k + 1$. We will give an example of two copies of ρ_F in $\mathcal{H}_2 \otimes \mathcal{H}_2$ which will show that this bound can be tight. The idea is again to use the $U \otimes U^*$ invariance of each copy of ρ_F. We show how to construct the density matrix $\rho_F^{\otimes 2}$ where ρ_F is a 2-qubit state at $F = \frac{1}{\sqrt{2}}$ by mixing Schmidt rank two vectors. Let $|\psi\rangle$ be the state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left[|0, \psi_0\rangle \otimes |0, \psi_0\rangle + |1, 0\rangle \otimes |1, 0\rangle \right], \quad (14)$$

where

$$|\psi_0\rangle = \sqrt{2}\sqrt{\sqrt{2} - 1}|0\rangle + (1 - \sqrt{2})|1\rangle. \quad (15)$$

This is a maximally entangled Schmidt rank two state between $\mathcal{H}_{A_1, A_2}$ and $\mathcal{H}_{B_1, B_2}$. Now Alice and Bob perform the following operations on this state:

- They perform the superoperator $\mathcal{S}^{U \otimes U^*}$, Eq. (9), on the Hilbert space $\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1}$ and they apply the same superoperator on $\mathcal{H}_{A_2} \otimes \mathcal{H}_{B_2}$.

- Then Alice and Bob symmetrize the state between system 1 and system 2, i.e. with probability $1/2$, they locally swap qubit $A_1 \leftrightarrow A_2$ and $B_1 \leftrightarrow B_2$ and with probability $1/2$ they do nothing.

By these two $LO + CC$ operations any initial state is mapped onto a state of the form

$$a \left(\mathbf{1} - |\Psi^+\rangle\langle\Psi^+| \right)^{\otimes 2} + b \, |\Psi^+\rangle\langle\Psi^+| \otimes \left[\mathbf{1} - |\Psi^+\rangle\langle\Psi^+| \right]$$
$$+ b \left[\mathbf{1} - |\Psi^+\rangle\langle\Psi^+| \right] \otimes |\Psi^+\rangle\langle\Psi^+| + c \left(|\Psi^+\rangle\langle\Psi^+| \right)^{\otimes 2} \quad (16)$$

By going through the algebra, one can check that the two operations on the state $|\psi\rangle$ result in $a = \frac{[\sqrt{2}-1]^2}{18}$, $b = \frac{\sqrt{2}-1}{6}$ and $c = \frac{1}{2}$. We have shown that the state $\rho_{F=\frac{1}{\sqrt{2}}}$ has Schmidt number two *and* $\rho_{F=\frac{1}{\sqrt{2}}}^{\otimes 2}$ has Schmidt number 2! This is an example of nonadditivity of the function $\mathcal{N}$ in Eq. (12). We have numerical evidence that the lower bound on the Schmidt number at $F = \frac{\sqrt{3}}{2}$ is tight as well, i.e. it seems possible to make $\rho_F^{\otimes 2}$ at $F = \frac{\sqrt{3}}{2}$ with mixing only Schmidt rank 3 vectors. The stepwise behavior of Schmidt number is illustrated in Figure 1.
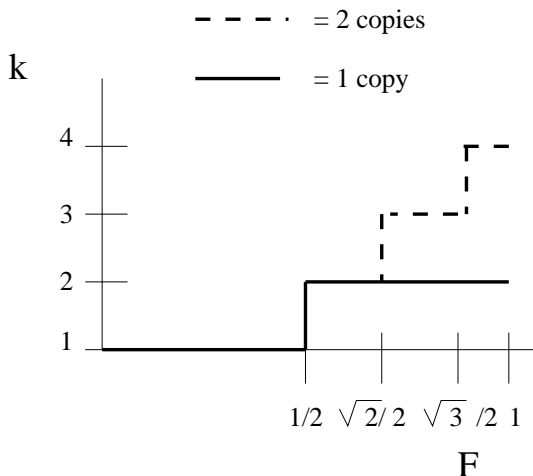
FIG. 1. The Schmidt number of one and two copies of ρ_F for $N = 2$ as a function of F.

Since we have found that the Schmidt number can exhibit 'nonadditivity', we can define the asymptotic Schmidt characteristic of a state

$$\mathcal{N}^{\infty}(\rho) = \lim_{m \to \infty} \left\{ \frac{\log k}{m} \; : \; \rho^{\otimes m} \text{ has Schmidt number } k \right\}. \tag{17}$$

The asymptotic Schmidt number of a density matrix gives us some information about whether two states, whose single copy Schmidt number is identical, can be interconverted by $LO + CC$. Say we have two density matrices ρ_1 and ρ_2 which each have Schmidt number k. But assume that for some n the Schmidt number of $\rho_1^{\otimes n}$ is larger than the Schmidt number of $\rho_2^{\otimes n}$. Then it follows that a single copy of ρ_2 cannot be converted by $LO+CC$ to ρ_2, because, if it could, then by repeating this procedure n times we could convert $\rho_2^{\otimes n}$ to $\rho_1^{\otimes n}$, which is in violation of Proposition 1.

In conclusion, we have introduced a new criterion for $LO + CC$ convertibility for bipartite mixed states and shown its relation to k-positive maps. Since the theory of k-positive maps is not (yet) greatly developed, we have not been able to use this connection extensively. We have found that Schmidt number for mixed states behaves differently than for pure states, in particular it does not necessarily increase when taking tensor copies of a state. This feature of 'nonadditivity' makes it possible to pose the following open question: Assume that a bipartite state ρ_1 has a higher Schmidt number than ρ_2, and thus ρ_2 cannot be converted to ρ_1. Assume however that for some ρ_{help} we can prove that $\rho_1 \otimes \rho_{help}$ and $\rho_2 \otimes \rho_{help}$ have the *same* Schmidt number or that $\rho_2 \otimes \rho_{help}$ has a larger Schmidt number. Then it could possibly be that $\rho_2 \otimes \rho_{help}$ can be converted to $\rho_1 \otimes \rho_{help}$. This would be an example of the use of borrowing of entanglement for mixed state conversions. Such a borrowing scheme has been found for exact pure state conversion [18]; it would

be interesting to see whether it is possible in the mixed state domain.

Proof of Theorem 1

Before proving Theorem 1 it will be useful to give some properties related to k-positivity and an alternative formulation of k-positivity:

Lemma 3 *The linear Hermiticity-preserving map Λ is k-positive if and only if*

$$(\mathbf{1} \otimes \Lambda)(|\Psi_k\rangle\langle\Psi_k|) \geq 0, \tag{18}$$

for all $|\Psi_k\rangle$ which are maximally entangled Schmidt rank k vectors. The linear Hermiticity-preserving map Λ is k-positive if and only if

$$\sum_{n,m=1}^{k} \sqrt{\mu_n \mu_m} \langle b_n| \Lambda(|a_n\rangle\langle a_m|) |b_m\rangle \geq 0, \tag{19}$$

for all possible orthogonal sets of vectors $\{|a_n\rangle\}_{n=1}^{k}$ and $\{|b_n\rangle\}_{n=1}^{k}$ and Schmidt coefficients $\{\mu_n\}$, $\sum_{n=1}^{k} \mu_n = 1$. Finally, if Λ is k-positive, then $\Lambda^{\dagger}$ defined by $\mathrm{Tr}\, A^{\dagger}\Lambda(B) = \mathrm{Tr}\, \Lambda^{\dagger}(A^{\dagger})B$ for all A and B, is also k-positive.

Proof (sketch) Equation (18) can be proved in a fashion completely analogous to Lemma 7 in Ref. [9]; there it is proved for $k = 2$. Equation (19) has been proved by A. Uhlmann [16] and can be understood as follows. It is equivalent to

$$\sum_{n,m,i,j=1}^{k} \sqrt{\mu_n \mu_m} \\ \langle \gamma_n, b_n| (\mathbf{1} \otimes \Lambda)(|\gamma_i, a_i\rangle\langle\gamma_j, a_j|)|\gamma_m, b_m\rangle \geq 0, \tag{20}$$

for any orthogonal set $\{|\gamma_n\rangle\}_{n=1}^{k}$, or

$$\langle\psi| (\mathbf{1} \otimes \Lambda)(|\Psi_k\rangle\langle\Psi_k|) |\psi\rangle \geq 0, \tag{21}$$

for arbitrary $|\psi\rangle$ and $|\Psi_k\rangle$. The k-positivity of $\Lambda^{\dagger}$ can be seen by noting that Eq. (2) can be written in terms of $\Lambda^{\dagger}$ as

$$\langle\psi| (\mathbf{1} \otimes \Lambda^{\dagger})(|\phi\rangle\langle\phi|) |\psi\rangle \geq 0, \tag{22}$$

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for all $|\psi\rangle\langle\psi| \in S_k$ and arbitrary $|\phi\rangle$. Since $|\psi\rangle$ has Schmidt rank k or less, it follows that we can restrict the state $|\phi\rangle$ to be of Schmidt rank k as well, or $|\phi\rangle\langle\phi| \in S_k$. $\square$

Proof of Theorem 1 Consider the "if" part of the theorem. Suppose, conversely, that there exist some ϱ of Schmidt number at most k for which at some time Eq. (3) is satisfied for some k-positive map Λ_k. The first assumption guarantees that ϱ is a convex combination of pure states $|\psi_i\rangle\langle\psi_i|$ of Schmidt rank at most k each. From the definition of k-positivity it follows immediately that all $|\psi_i\rangle\langle\psi_i|$ remain positive after the action of $\mathbf{1}\otimes\Lambda_k$, so their convex combination equal to ϱ remains positive too. But this then is in a contradiction with Eq. (3).

Consider the "only if" part of the theorem. Let ρ have Schmidt number at least $k + 1$, i.e. $\rho \notin S_k$. Then there exists a hyperplane $\{\sigma \in S \,|\, \mathrm{Tr}\, H\sigma = 0\}$ which separates the convex compact set S_k and the point $\rho \notin S_k$, i.e. there exists a Hermitian operator H such that

$$\mathrm{Tr}\, H\rho < 0 \ \text{ and } \ \forall \sigma \in S_k \ \mathrm{Tr}\, H\sigma \geq 0. \qquad (23)$$

We will show that we can associate with this Hermitian operator H a positive linear map Λ_k which is k-positive. We define Λ as

$$H = (\mathbf{1} \otimes \Lambda_k)(|\Psi^+\rangle\langle\Psi^+|), \qquad (24)$$

where $|\Psi^+\rangle = \frac{1}{\sqrt{n}} \sum_{i=1}^n |ii\rangle$. We use $\mathrm{Tr}\, H\sigma \geq 0$ where we take σ to be an entangled Schmidt rank k vector, $\sigma = \sum_{n,m=1}^k \sqrt{\lambda_m\lambda_n}|a_m, b_m\rangle\langle a_n, b_n|$. We will denote transposition in the full $\{|a_n\rangle\}$ basis as T^a. We can rewrite the expression

$$\sum_{n,m=1}^k \sqrt{\lambda_m\lambda_n}\,\mathrm{Tr}\, H\,|a_m, b_m\rangle\langle a_n, b_n| \geq 0, \qquad (25)$$

using Eq. (24) and the expansion of a linear map $\mathcal{S}$ on an operator X as $\mathcal{S}(X) = \sum_{i,j=1}^n \langle i|X|j\rangle\mathcal{S}(|i\rangle\langle j|)$, as

$$\frac{1}{n} \sum_{m,n=1}^k \sqrt{\lambda_n\lambda_m}\langle b_n|\,\Lambda_k \circ T \circ T^a(|a_n\rangle\langle a_m|)\,|b_m\rangle \geq 0. \qquad (26)$$

Lemma 3 then implies that the map $\Lambda_k \circ T \circ T^a$ is k-positive. The map $T \circ T^a$ maps the vector $|a_n\rangle$ onto $|a_n^*\rangle$ where complex conjugation is performed with respect to the $\{|i\rangle\}$ basis. This corresponds to a unitary rotation from the $\{|a_n\rangle\}$ basis to the $\{|a_n^*\rangle\}$ basis. Therefore Λ_k itself will be k-positive. On the other hand the condition $\mathrm{Tr}\, H\rho < 0$ can be rewritten, using Eq. (24), as

$$\langle\Psi^+|\,(\mathbf{1} \otimes \Lambda_k^\dagger)(\rho)\,|\Psi^+\rangle < 0. \qquad (27)$$

Since Λ_k is k-positive, $\Lambda_k^\dagger$ is k-positive, see Lemma 3. This completes the proof. $\square$

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