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Hermitian Schmidt decomposition and twin observables of bipartite mixed states

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Abstract
The study of mixed-state quantum correlations in terms of opposite-subsystem observables—the measurement of one of which amounts to the same as that of the other—of so-called twins is continued. Twin events that imply biorthogonal mixing of states, called 'strong twin events', are studied. It is shown that for each mixed state there exists a Schmidt (super-state-vector) decomposition in terms of Hermitian operators, and that it can be the continuation of the above-mentioned biorthogonal mixing due to strong twins. The case of weak twins and non-Hermitian Schmidt decomposition is also investigated. For separable states a necessary and sufficient condition for the existence of nontrivial twins is derived. Utilization of the Hermitian Schmidt decomposition for finding all twins is illustrated in full detail for the case of the two spin-half-particle states with maximally disordered subsystems (mixtures of Bell states). It is shown that only rank-two mixtures have nontrivial twins.

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1. Introduction

Nowadays one distinguishes sharply between separable bipartite mixtures, which are quasiclassically correlated, and nonseparable ones, endowed with entanglement, a purely quantum property. (A good example of the latter is the case of correlated pure states.) The term 'quantum correlations' is used in the generic sense, comprising both quasiclassical correlations and entanglement.

It was claimed in a recent investigation [1] that the study of quantum correlations through twin observables, or for short *twins*, is expected to be important for quantum communication and quantum information theories because it is believed to reveal some basic properties of the correlations. Twin observables are opposite-subsystem observables such that the (subsystem) measurement of one of them amounts *ipso facto* to a measurement also of the other. Equivalently put, the subsystem measurement of a twin gives rise, on account of the quantum correlations, to an orthogonal decomposition of the state of the opposite subsystem.

In bipartite mixed states it is easier to *relate twins to quantum correlations* than to entanglement (though the latter is more important). A quantitative measure of the former is what is called von Neumann's mutual information:

$$C(\rho_{12}) \equiv S(\rho_{12}|\rho_1 \otimes \rho_2) = S(\rho_1) + S(\rho_2) - S(\rho_{12})$$

expressed in terms of the so-called relative (or conditional) entropy, and, alternatively, in terms of the von Neumann entropies of the reduced statistical operators ρ_i, $i = 1, 2$ (subsystem states), and the von Neumann entropy of the statistical operator (bipartite state) ρ_{12} itself. I denote it by 'C' because it was thus designated and called the 'logarithmic correlation' by Lindblad [2]. He also made use of the classical discrete mutual information $I(A, B|\rho_{12})$ of two arbitrary opposite-subsystem observables A and B (with purely discrete spectra) which were assumed to be simultaneously measured in a quantum state ρ_{12}. Then, utilizing the spectral forms and the ensuing probabilities,

$$A = \sum_k a_k P_1^{(k)} \quad k \neq k' \Rightarrow a_k \neq a_{k'} \qquad B = \sum_l b_l Q_2^{(l)} \quad l \neq l' \Rightarrow b_l \neq b_{l'}$$

$$p(k, l) \equiv \mathrm{Tr}[\rho_{12}(P_1^{(k)} \otimes Q_2^{(l)})] \qquad p_k \equiv \sum_l p(k, l) \qquad p_l \equiv \sum_k p(k, l)$$

one defines the mutual information

$$H(A : B|\rho_{12}) \equiv H(p(k, l)|p_k p_l) = H(p_k) + H(p_l) - H(p(k, l))$$

where $H(p_k)$, e.g., is the so-called Gibbs–Boltzmann–Shannon entropy $H(p_k) \equiv -\sum_k p_k \log p_k$, etc. Finally, Lindblad defined

$$I(A, B|\rho_{12}) \equiv \sup H(A : B|\rho_{12})$$

where the *supremum* was taken over all possible choices of the observables.

Lindblad showed that

$$I(A, B|\rho_{12}) \leqslant C(\rho_{12})$$

and

$$C(\rho_{12}) > 0 \Rightarrow I(A, B|\rho_{12}) > 0$$

are always valid.

Thus, in all correlated states, i.e., in states in which $C(\rho_{12}) > 0$, or equivalently, $\rho_{12} \neq \rho_1 \otimes \rho_2$, one can understand part of the quantum correlations in terms of simultaneous subsystem measurements and their maximal mutual information.

Now, twins occupy a very special position among the subsystem observables, because if A and B are twins, then

$$I(A, B|\rho_{12}) = H(p_k)$$

since $H(p_k) = H(p_l) = H(p(k, l))$ due to the relation $p(k, l) = p_k \delta_{l, f(k)}$, where $f(k)$ is a fixed bijection of the values of k onto those of l. This is the case of *perfect correlations*, called the 'lossless and noiseless information channel' in information theory.

The investigation of *twins* began with *pure states* [3, 4] $\rho_{12} \equiv |\Phi\rangle\langle\Phi|$. Surprisingly, a necessary and sufficient condition for a subsystem observable A to have a nontrivial twin was found in terms of properties of ρ_1 alone (local properties; cf (2*a*)). The opposite-subsystem observable B that is the twin of A was, naturally, expressed in terms of global properties of $|\Phi\rangle$. These were in a simple way given in terms of an operator (called the correlation operator;

cf (11)) mapping the range of ρ_1 onto that of ρ_2. It was defined by $|\Phi\rangle$. This operator is most practically handled in terms of the so-called *Schmidt decomposition* [5] because it is precisely the (antiunitary) operator determining which characteristic vector of ρ_2 should appear in the same term as that of ρ_1 in the above-mentioned decomposition [3] (cf (11)).

When twins were investigated in *the mixed-state case* [1], the above-mentioned condition (cf (2a)) was found to be only necessary. In fact, a sufficient condition for A to have a twin expressed as a property of ρ_1 alone (a local property) cannot exist, because for every ρ_1 there is the uncorrelated state $\rho_{12} \equiv \rho_1 \otimes \rho_2$, which does not have nontrivial twins.

Thus, global properties inherent in ρ_{12} have to be made use of at the above-mentioned very first stage of investigation of twins in the mixed-state case. It is not easy to 'extract' a minimal global property of ρ_{12} that 'does the job' (as in the pure-state case).

It is a striking fact that the Schmidt decomposition of state vectors can be generalized to *all mixed states*. It is the basic aim of this paper to investigate the relevance of this decomposition to twins. It is proved that the Schmidt decomposition of *any bipartite mixed state* ρ_{12} need not be expressed in terms of some very general linear operators; it can be given exclusively in terms of Hermitian operators, which can, in principle, be physically interpreted as observables (cf theorem 2 and corollary 1).

The concept of strong twins, which are closely connected with biorthogonal decomposition of ρ_{12} (cf theorem 1), is introduced as a step towards the above-mentioned Hermitian Schmidt decomposition of ρ_{12}. Also non-Hermitian Schmidt decomposition of mixed states is studied (cf theorem 3).

For mixtures of Bell states a Hermitian Schmidt decomposition is given in the literature (though not treated as such). In this simple example the problem of finding *all twins* is easily solved (cf theorems 5 and 6)—in order to illustrate the relevance of the Hermitian Schmidt decomposition to extracting the sought-for global property inherent in ρ_{12}.

In the above-mentioned simple case it turns out that rank-four mixtures do not allow nontrivial twins. This is not surprising because it was shown in the preceding study [1] that singularity of ρ_{12} is a necessary condition. But, surprisingly, rank-three mixtures are shown to also have no nontrivial twins. This suggests that perhaps a stronger necessary condition, some kind of 'sufficient singularity', for the existence of nontrivial twins could be found in the general case. This will be followed up elsewhere.

Relating twins to *separability* is fully clarified in this study in terms of a necessary and sufficient condition for the existence of nontrivial twins (cf theorem 4). Relating twins to entanglement in the mixed-state case, and to the quantitative measures of entanglement like the so-called entanglement of creation and entanglement of distillation [6], or the quantum relative entropy [7] and others is an important open question that will be, we hope, treated in further work.

The study of twins pursued in a number of articles mentioned above is an *ab ovo* approach, which has already proved to be, in principle, relevant and perhaps even important to quantum information theory. It stands somewhat apart from the mainstream investigations. But it will be, we hope, connected up with the latter as a result of further exploration.

2. Preliminary relations

When a general, i.e., mixed or pure, bipartite state (statistical operator) ρ_{12} is given, twins (A_1, A_2) are algebraically defined as Hermitian (opposite-subsystem) operators satisfying

$$A_1\rho_{12} = A_2\rho_{12} \tag{1}$$

where A_1 is actually $(A_1 \otimes I_2)$, I_2 being the identity operator for the second subsystem, etc. It has been shown [1] that (1) implies

$$[A_1, \rho_1] = 0 \tag{2a}$$

$$[A_2, \rho_2] = 0 \tag{2b}$$

for the subsystem states (the reduced statistical operators) $\rho_1 \equiv \mathrm{Tr}_2\, \rho_{12}$, $\rho_2 \equiv \mathrm{Tr}_1\, \rho_{12}$. (The symbols Tr_i, $i = 1, 2$, denote the partial traces.) Relation $(2a)$ is the above-mentioned local necessary condition for A_1 to have a twin.

If P_1 is a first-subsystem projector, one can decompose the statistical operator:

$$\rho_{12} = P_1\rho_{12} + P_1^{\perp}\rho_{12} \tag{3}$$

where $P_1^{\perp}$ is the orthocomplementary projector of P_1. Let (P_1, P_2) be a pair of nontrivial twin events (twin projectors) for ρ_{12}. In general, the terms on the RHS are not even Hermitian. First, we are going to investigate the more important case where (3) is *a mixture of states*.

3. Strong twin projectors and biorthogonal mixtures

Let (P_1, P_2) be a pair of nontrivial twin projectors for a composite-system statistical operator ρ_{12}.

Remark 1. Evidently, either both terms on the RHS of (3) are Hermitian or neither of them is. They are *Hermitian* if and only if the projector P_1 (or equivalently, $P_1^{\perp}$) *commutes* with ρ_{12}:

$$[P_i, \rho_{12}] = 0 \qquad i = 1, 2 \tag{4}$$

(any one of the equalities implies the other), as seen by adjoining the terms in (3).

Hermiticity of the terms in (3) implies that they are statistical operators (up to normalization constants), i.e., that (3) is *a mixture*. That is, if (4) is valid, then idempotency leads to $P_1\rho_{12} = P_1\rho_{12}P_1$, which is evidently a positive operator. Since

$$\mathrm{Tr}\, P_1\rho_{12}P_1 \leqslant \mathrm{Tr}\, \rho_{12} = 1$$

the operator has a finite trace.

Definition 1. *Nontrivial twin events (projectors) we call either strong twin events (projectors), if they satisfy (4), or weak twin events (projectors), if (4) is not satisfied.*

A strong twin event P_1 implies a mixture (3) of states that have a strong property called biorthogonality. To understand it, we first recall the (ordinary) orthogonality of states.

If ρ' and ρ'' are statistical operators with Q' and Q'' as their respective range projectors, then one has the known equivalences

$$\rho'\rho'' = 0 \Leftrightarrow Q'Q'' = 0 \Leftrightarrow \mathcal{R}(\rho') \perp \mathcal{R}(\rho'') \tag{5}$$

where the last relation expresses the orthogonality of the ranges.

Any of the three relations in (5) defines the *orthogonality of states*.

Definition 2. *If*

$$\rho_{12} = w\rho'_{12} + (1-w)\rho''_{12} \qquad 0 < w < 1 \tag{6}$$

is a mixture of states such that

$$\rho'_i\rho''_i = 0 \qquad i = 1, 2 \tag{7}$$

where $\rho'_1 \equiv \mathrm{Tr}_2\, \rho'_{12}$ *etc are the reduced statistical operators, then we say that (6) is a biorthogonal mixture.*

To prove a close connection between strong twin events and biorthogonal mixtures, we need another known general property of composite-system statistical operators ρ_{12}:

$$\rho_{12} = Q_1\rho_{12} = \rho_{12}Q_1 = Q_2\rho_{12} = \rho_{12}Q_2 \quad (8)$$

where Q_i is the range projector of the corresponding reduced statistical operator ρ_i, $i = 1, 2$.

Theorem 1. *If P_1 is a nontrivial twin event, expression (3) is a biorthogonal mixture if and only if P_1 is a strong twin event.*

Proof. *Sufficiency.* If P_1 is a strong twin projector and (6) is obtained by rewriting (3), then $\rho'_{12} = P_1\rho'_{12}$ is valid, and this implies $\rho'_1 = P_1\rho'_1$ for the reduced statistical operator, and, adjoining this, one arrives at $\rho'_1 = \rho'_1 P_1$. On the other hand, one has analogously $\rho''_{12} = P_1^{\perp}\rho''_{12}$ implying $\rho''_1 = P_1^{\perp}\rho''_1$. Finally,

$$\rho'_1\rho''_1 = (\rho'_1 P_1)(P_1^{\perp}\rho''_1) = 0.$$

The symmetrical argument holds for the second tensor factor.

Necessity. If (6) is a biorthogonal mixture, then we define $P_i \equiv Q'_i$, $i = 1, 2$, i.e., we take the range projectors of the reduced statistical operators of ρ'_{12} as candidates for our twin projectors. On account of (8), we can write (6) as follows:

$$\rho_{12} = wQ'_1Q'_2\rho'_{12}Q'_1Q'_2 + (1-w)Q''_1Q''_2\rho''_{12}Q''_1Q''_2.$$

Since, in view of (5), biorthogonality (7) implies $Q'_iQ''_i = 0$, $i = 1, 2$, it is now obvious that P_1 and P_2, multiplying ρ_{12} from the left, give one and the same operator, i.e., that they are twins, and it is also obvious that they both give the same operator irrespective of whether they multiply ρ_{12} from the left or from the right, i.e., that they are strong twin projectors. □

In view of (5), it is clear that biorthogonal decomposition of a statistical operator can be, in principle, *continued*: if, e.g., ρ'_{12} in the biorthogonal decomposition (6) is, in its turn, decomposed into biorthogonal statistical operators and replaced in (6), then any two of the new terms are biorthogonal, etc.

An extreme case of a biorthogonal mixture is a *separable* one:

$$\rho_{12} = \sum_k w_k(\rho_1^{(k)} \otimes \rho_2^{(k)}) \quad (9)$$

where

$$\forall k: \qquad w_k > 0 \quad \rho_i^{(k)} > 0 \quad \mathrm{Tr}\,\rho_i^{(k)} = 1 \quad (i = 1, 2) \qquad \sum_k w_k = 1$$

('$\rho > 0$' denotes positivity of the operator). This decomposition cannot, of course, always be carried out, but examples are well known. For instance, if one performs ideal nonselective measurement of the z-component of spin of the first particle in a singlet two-particle state, one ends up with

$$\rho_{12} \equiv (1/2)(|z+\rangle_1\langle z+|_1 \otimes |z-\rangle_2\langle z-|_2 + |z-\rangle_1\langle z-|_1 \otimes |z+\rangle_2\langle z+|_2).$$

This is obviously a biorthogonal separable mixture.

One might wonder whether, at the price of relaxing the requirement of statistical operator terms as slightly as possible, there could exist a *general* decomposition into *uncorrelated* terms (like in (9)).

To find a definite answer to this, we consider the known case of general (entangled or disentangled) composite-system *state vectors* and their Schmidt decompositions. Let us summarize the relevant information on this in sufficient detail [3].

The Schmidt decomposition of an arbitrary pure-state vector $|\Phi\rangle_{12}$ of a composite system is expressed in terms of *its canonical entities*. They are the following:

(i) *The reduced statistical operators* (subsystem states) ρ_1 ($\equiv \mathrm{Tr}_2\, |\Phi\rangle_{12}\langle\Phi|_{12}$) and ρ_2 (defined symmetrically) are well known.

(ii) The spectral forms of the reduced statistical operators are

$$\rho_1 = \sum_i r_i |i\rangle_1\langle i|_1 \qquad \forall i\colon r_i > 0 \tag{10a}$$

$$\rho_2 = \sum_i r_i |i\rangle_2\langle i|_2 \qquad \forall i\colon r_i > 0. \tag{10b}$$

(Note that the positive spectra—multiplicities included—are always equal.)

(iii) Finally, the above-mentioned expansion utilizes the (antiunitary) *correlation operator* U_a, which maps the range $\mathcal{R}(\rho_1)$ onto the range $\mathcal{R}(\rho_2)$. (Note that they are always equally dimensional in the pure-state case.) The correlation operator is determined by $|\Phi\rangle_{12}$, and, in turn, in conjunction with ρ_1, it determines $|\Phi\rangle_{12}$.

The *Schmidt decomposition* reads

$$|\Phi\rangle_{12} = \sum_i r_i^{1/2} |i\rangle_1 \otimes (U_a|i\rangle_1)_2. \tag{11}$$

The normalized characteristic vectors $|i\rangle_2$ in (10b) may (but need not) be chosen to be equal to $(U_a|i\rangle_1)_2$.

In case of a state vector $|\Phi\rangle_{12}$, the characteristic relation (1) for twins reduces to

$$A_1|\Phi\rangle_{12} = A_2|\Phi\rangle_{12}. \tag{12}$$

The corresponding twin A_2 then satisfies

$$A_2 = U_a A_1 U_a^{-1} Q_2 + A_2 Q_2^{\perp} \tag{13}$$

where Q_2 is the range projector of ρ_2, and $Q_2^{\perp}$, its orthocomplementary projector, projects onto the null space of ρ_2.

One should note that, on account of the commutation (2b), both the range and the null space of ρ_2 are invariant for A_2. Further, the second term on the RHS of (13), or rather the restriction of A_2 to the null space, which corresponds to it, is completely arbitrary and immaterial for the twin property (12), because it acts as zero on $|\Phi\rangle_{12}$. (Naturally, the symmetric claim holds true for A_1 and ρ_1.)

4. Hermitian Schmidt decomposition of bipartite statistical operators

It is well known that linear Hilbert–Schmidt operators A acting in a Hilbert space, i.e., those with a finite Hilbert–Schmidt norm $(\mathrm{Tr}\, A^\dagger A)^{1/2}$, form a Hilbert space in their turn. Writing the operator A as a (Hilbert–Schmidt) super-vector $|A\rangle$, the scalar product is

$$\langle A||B\rangle \equiv \mathrm{Tr}\, A^\dagger B.$$

Since for every statistical operator ρ, one has $\mathrm{Tr}\,\rho^2 \leqslant 1$, it is a Hilbert–Schmidt operator. Therefore, *every statistical operator has a Schmidt decomposition*.

The trouble is that the operators that take the place of the state-vector tensor factors in the terms of (11), which are the sought-for generalizations of the statistical operators $\rho_i^{(k)}$, $i = 1, 2$, in (9), are in general linear operators. This might be too wide a generalization. One might wonder whether it could be confined to Hermitian operators.

When we view the operators as super-vectors, then we must view *adjoining* of operators as *an antiunitary* operator whose square is the identity operator, i.e., which is an *involution*.

Hence, we denote adjoining by $V_1^{(a)} \otimes V_2^{(a)}$ for a composite system. The operators that are *invariant* under the action of this antiunitary involution are Hermitian.

Fortunately, the Schmidt decomposition can always be expressed in terms of Hermitian operators. We put this in a more precise and a more detailed way. But it is simpler to return to the Hilbert space of state vectors for some elaboration.

Theorem 2. *Let $V_1^{(a)} \otimes V_2^{(a)}$ be a given antiunitary involution acting on composite-system state vectors. One has the equivalence*

$$(V_1^{(a)} \otimes V_2^{(a)})|\Phi\rangle_{12} = |\Phi\rangle_{12} \Leftrightarrow [\rho_i, V_i^{(a)}] = 0 \quad (i = 1, 2) \qquad V_2^{(a)} U_a V_1^{(a)} = U_a \tag{14}$$

where ρ_i, U_a are the above-mentioned canonical entities of $|\Phi\rangle_{12}$. (Note that in the last relation we actually have the restriction of $V_1^{(a)}$ to $\mathcal{R}(\rho_1)$.)

Proof. Let $|\Phi\rangle_{12}$ be invariant under the action of the antiunitary involution. Then

$$\begin{aligned} V_1^{(a)} \rho_1 V_1^{(a)} &= V_1^{(a)} (\mathrm{Tr}_2 |\Phi\rangle_{12}\langle\Phi|_{12}) V_1^{(a)} \\ &= \mathrm{Tr}_2 (V_1^{(a)} |\Phi\rangle_{12}\langle\Phi|_{12} V_1^{(a)}) \\ &= \mathrm{Tr}_2 \{V_1^{(a)} [(V_1^{(a)} \otimes V_2^{(a)}) |\Phi\rangle_{12}\langle\Phi|_{12} (V_1^{(a)} \otimes V_2^{(a)})] V_1^{(a)}\} \\ &= \mathrm{Tr}_2 (V_2^{(a)} |\Phi\rangle_{12}\langle\Phi|_{12} V_2^{(a)}) = \mathrm{Tr}_2 |\Phi\rangle_{12}\langle\Phi|_{12} = \rho_1 \end{aligned}$$

and symmetrically for ρ_2. It should be noted that an antiunitary involution equals its inverse and its adjoint. Further, use has been made of some known basic properties of partial traces (which are analogous to the well known ones for ordinary traces).

Commutation of ρ_1 with the antiunitary involution $V_1^{(a)}$ allows one to choose the characteristic basis $\{|i\rangle_1 : \forall i\}$ of the former spanning its range consisting of vectors invariant under the action of $V_1^{(a)}$ (cf [8]).

Now, let us take the Schmidt decomposition (11) in terms of such an invariant basis. Then

$$(V_1^{(a)} \otimes V_2^{(a)})|\Phi\rangle_{12} = \sum_i r_i^{1/2} |i\rangle_1 \otimes V_2^{(a)} (U_a |i\rangle_1)_2.$$

Since $|\Phi\rangle_{12}$ is assumed to be invariant, it follows that also

$$|\Phi\rangle_{12} = \sum_i r_i^{1/2} |i\rangle_1 \otimes V_2^{(a)} (U_a |i\rangle_1)_2.$$

The second tensor factor in each term is uniquely determined by the LHS and the corresponding first tensor factor (as a partial scalar product; cf [3]). Comparison with (11) then shows that

$$\forall i: \qquad V_2^{(a)} U_a |i\rangle_1 = U_a |i\rangle_1.$$

Since $|i\rangle_1 = V_1^{(a)} |i\rangle_1$, we further have

$$V_2^{(a)} U_a V_1^{(a)} = U_a$$

as claimed.

Conversely, if the main canonical entities are in the relation to the antiunitary involutions stated in (14), then we can expand $|\Phi\rangle_{12}$ in a characteristic basis in ρ_1 spanning its range that is invariant under the antilinear operator. Then (11) immediately reveals that, as a consequence, $|\Phi\rangle_{12}$ is invariant under $V_1^{(a)} \otimes V_2^{(a)}$. □

Corollary 1. *Every composite-system statistical operator ρ_{12} has, after super-vector normalization, a Hermitian Schmidt decomposition.*

Proof. Since every ρ_{12}, being Hermitian, is invariant under the antiunitary involution $V_1^{(a)} \otimes V_2^{(a)}$, it is clear from the proof of theorem 2 that ρ_{12}, upon super-vector normalization, has a Schmidt decomposition in terms of Hermitian operators. □

Returning to a biorthogonal mixture, one might wonder if one can *continue* such a decomposition by writing each term in a Hermitian Schmidt decomposition in order to obtain the latter decomposition for the entire statistical operator. The answer is affirmative on account of the following.

Going back to (5), we can add a fourth equivalent property.

Proposition 1. *Two statistical operators ρ' and ρ'' are orthogonal if and only if they are orthogonal as Hilbert–Schmidt super-vectors.*

Proof. It is obvious that orthogonality (in the sense of (5)) implies Hilbert–Schmidt orthogonality. To see the converse implication, we make use of the fact that every statistical operator has a purely discrete spectrum [9], and we decompose the statistical operators in terms of characteristic vectors corresponding to positive characteristic values:

$$\langle \rho' || \rho'' \rangle = \mathrm{Tr}\, \rho' \rho'' = \mathrm{Tr} \sum_k r_k |k\rangle\langle k| \sum_j \bar{r}_j |j\rangle\langle j| = \sum_k \sum_j r_k \bar{r}_j |\langle j||k\rangle|^2.$$

Hence,

$$\langle \rho' || \rho'' \rangle = 0 \Rightarrow \rho' \rho'' = 0$$

(cf the third relation in (5)). □

If (A_1, A_2) is a pair of *twin observables*, then the detectable parts A_i', $i = 1, 2$, have a common purely discrete spectrum $\{a_n : \forall n\}$ (with, in general, different multiplicities), and the corresponding (detectable) characteristic projectors $\{P_i^{(n)} : i = 1, 2, \forall n\}$, are also pairs of twins [1].

Definition 3. *If all above-mentioned characteristic projector pairs $(P_1^{(n)}, P_2^{(n)})$ are strong twin projectors, then (A_1, A_2) is a pair of strong twin observables. If some of the detectable characteristic twin projectors are strong and some weak, we say that we have partially strong (or, synonymously, partially weak) twin observables. If all the above-mentioned twin projectors are weak, then we have a weak pair of twin observables.*

A pair (A_1, A_2) of nontrivial twin observables for ρ_{12} is a pair of strong ones if and only if

$$[A_i, \rho_{12}] = 0 \qquad i = 1, 2 \tag{15}$$

is valid. This is so because commutation with all characteristic projectors is equivalent to commutation with the Hermitian operator itself, and, if P_1 (e.g.) is a nondetectable characteristic projector of A_1, then one has commutation because

$$P_1 \rho_{12} = (P_1 Q_1^{\perp}) \rho_{12} = 0 = \rho_{12} (Q_1^{\perp} P_1) = \rho_{12} P_1$$

on account of (8).

Strong twin observables, by means of their strong characteristic twin projectors, lead to a generalization of (3):

$$\rho_{12} = \sum_n P_1^{(n)} \rho_{12} = \sum_n w_n \rho_{12}^{(n)} \tag{16a}$$

where

$$\forall n: \qquad w_n \equiv \mathrm{Tr}\, \rho_{12} P_1^{(n)} \qquad \rho_{12}^{(n)} \equiv (w_n)^{-1} P_1^{(n)} \rho_{12}. \tag{16b}$$

Naturally, if $P_1^{(n)}\rho_{12} = 0$, then $\rho_{12}^{(n)}$ is not defined. Any two terms in (16a) are biorthogonal.

Note that we utilize the entire characteristic projectors, which are the orthogonal sums of the detectable and the nondetectable parts: $P_1^{(n)} = (P_1')^{(n)} \oplus (P_1'')^{(n)}$ paralleling $\mathcal{H}_1 = \mathcal{R}(\rho_1) \oplus \mathcal{R}^{\perp}(\rho_1)$. We can do this because $(P_1')^{(n)}\rho_{12} = P_1^{(n)}\rho_{12}$.

Proposition 2. *If*

$$\rho_1^{(n)} \equiv \mathrm{Tr}_2\, \rho_{12}^{(n)}$$

(and symmetrically for $\rho_2^{(n)}$) are the reduced statistical operators of the terms in a biorthogonal mixture (16a), then

$$P_i^{(n)}\rho_i^{(n)} = \rho_i^{(n)} \qquad i = 1, 2 \tag{17a}$$

or, equivalently,

$$\mathcal{R}(\rho_i^{(n)}) \subseteq \mathcal{R}(P_i^{(n)}) \qquad i = 1, 2. \tag{17b}$$

Proof. On account of the definition of (16a), one has $P_i^{(n)}\rho_{12}^{(n)} = \rho_{12}^{(n)}$. Taking the opposite-subsystem partial trace, one obtains $P_i^{(n)}\rho_i^{(n)} = \rho_i^{(n)}$ $i = 1, 2$. □

Corollary 2. *If the detectable part A_1' of a twin observable A_1 has a nondegenerate characteristic value a_n corresponding to a strong characteristic twin projector $(P_1')^{(n)} = |\,\psi^{(n)}\,\rangle_1\langle\,\psi^{(n)}\,|_1$, $|\,\psi^{(n)}\,\rangle_1 \in \mathcal{R}(\rho_1)$, then the term in the biorthogonal mixture (16a) that corresponds to it has the form*

$$w_n|\,\psi^{(n)}\rangle_1\langle\psi^{(n)}\,|_1 \otimes \rho_2^{(n)} \tag{18}$$

where $\rho_2^{(n)}$ is a (second-subsystem) statistical operator and (18) is a term in a final Hermitian Schmidt decomposition of ρ_{12}.

Any biorthogonal decomposition of a composite-system statistical operator ρ_{12} (into two or more terms) can be continued in each term separately into a Schmidt decomposition of ρ_{12} in terms of Hermitian operators.

The biorthogonal decomposition is *an intermediate step*. This is similar to the case where we can partially diagonalize the Hamiltonian of a quantum system (due to some symmetry, e.g.). The diagonalization is then continued separately with each submatrix on the diagonal of the Hamiltonian.

The continuation from a biorthogonal mixture to a Hermitian Schmidt decomposition can always be performed, in principle, 'by brute force': diagonalizing the reduced statistical super-operator $\hat{\rho}_1$ of the normalized super-vector $|\,\rho_{12}\,\rangle$ (analogously to how it is done for an ordinary state vector), and by finding an invariant basis for $V_1^{(a)}$ in each characteristic subspace thus obtained [8].

5. Weak twins and non-Hermitian Schmidt decomposition

For the sake of completeness, it is desirable to investigate decomposition (3) also for a weak nontrivial twin projector P_1. First, we take an analytical view of theorem 1 and realize that the biorthogonality of the two terms in (3) is connected with the twin property (strong or weak), and the strong twin property corresponds to the hermiticity of the terms. Let us put this more precisely.

Remark 2. A decomposition

$$\rho_{12} = A_{12} + B_{12}$$

of a composite-system statistical operator ρ_{12} into two linear operators is *biorthogonal* if there exist two opposite-subsystem projectors (P_1, P_2) such that

$$A_{12} = P_1 A_{12} = P_2 A_{12} \qquad 0 = P_1 B_{12} = P_2 B_{12}$$
$$0 = P_1^{\perp} A_{12} = P_2^{\perp} A_{12} \qquad B_{12} = P_1^{\perp} B_{12} = P_2^{\perp} B_{12}.$$

It is clear from theorem 1 that any biorthogonal mixture (of states) (6) satisfies the condition given in remark 2. Having in mind (3), it is also evident that biorthogonality is equivalent to the existence of a pair of twin projectors (weak or strong). Finally, the strength property of the twins is equivalent to the hermiticity of the terms in (3), which results in there being statistical operator terms (and a mixture).

Theorem 3. *If (P_1, P_2) is a pair of weak twin projectors for a composite-system statistical operator ρ_{12}, then the terms in (3) are super-vectors, and replacing each by a (non-Hermitian) Schmidt decomposition, one obtains a decomposition of the same kind for the entire statistical operator.*

Proof. Since in

$$1 \geqslant \mathrm{Tr}\, \rho_{12}^2 = \mathrm{Tr}\, \rho_{12} P_1 \rho_{12} + \mathrm{Tr}\, \rho_{12} P_1^{\perp} \rho_{12}$$

the terms are non-negative (as traces of positive operators), the terms in (3) are Hilbert–Schmidt operators, i.e., super-vectors. Suppose that we have decomposed the first term in (3) in the Schmidt way:

$$P_1 \rho_{12} = c \sum_i r_i^{1/2} A_1^{(i)} \otimes B_2^{(i)}$$

where c is a normalization constant (because the statistical operator is not a super-state vector unless it is a pure state). Since the LHS is invariant under P_1, so is each first-subsystem linear operator $A_1^{(i)}$, because the second factors in the expansion have unique corresponding first factors. If we decompose also the second term in (3) in the Schmidt way:

$$P_1^{\perp} \rho_{12} = c' \sum_j r_j'^{1/2} C_1^{(j)} \otimes D_2^{(j)}$$

then, analogously, invariance of each factor $C_1^{(j)}$ under $P_1^{\perp}$ follows. This results in super-vector orthogonality:

$$\forall i, j: \qquad \mathrm{Tr}[(A_1^{(i)})^{\dagger} C_1^{(j)}] = \mathrm{Tr}[(A_1^{(i)})^{\dagger} P_1 P_1^{\perp} C_1^{(j)}] = 0.$$

A symmetrical argument applies for the second factors and P_2. Thus, replacing both terms in (3) by their non-Hermitian Schmidt decompositions, we have biorthogonality between any term of the first decomposition and any term of the second one. Therefore, we have a decomposition of the same kind of the whole of ρ_{12}. □

It is now clear that in the case of weak twin projectors also the decomposition (3) can be *continued*, but this time *to a non-Hermitian Schmidt decomposition*.

A non-Hermitian Schmidt decomposition need not be wild and far fetched from the physical point of view. Let me illustrate this by the obvious fact that a Schmidt decomposition of a state vector $|\Phi\rangle_{12}$:

$$|\Phi\rangle_{12} = \sum_i r_i^{1/2} |i\rangle_1 |i\rangle_2 \qquad \langle i|_p |i'\rangle_p = \delta_{i,i'} \quad p = 1, 2$$

immediately results in a non-Hermitian Schmidt decomposition of the statistical operator $|\Phi\rangle_{12}\langle\Phi|_{12}$:

$$|\Phi\rangle_{12}\langle\Phi|_{12} = \sum_i \sum_{i'} r_i^{1/2} r_{i'}^{1/2} |i\rangle_1 \langle i'|_1 \otimes |i\rangle_2 \langle i'|_2.$$

Finally, let us return to separable mixtures.

6. Nontrivial twin projectors for separable mixtures

Let (9) be a general separable mixture. Let us clarify under what conditions it has nontrivial twin events.

Theorem 4. *A general separable mixture (9) has a nontrivial twin projector P_1 if and only if the set of all values of the index 'k' is the union of two nonoverlapping subsets, say, consisting of 'k''-values and of 'k'''-values respectively, and, when (9) is rewritten accordingly:*

$$\rho_{12} = \sum_{k'} w_{k'} \rho_1^{(k')} \otimes \rho_2^{(k')} + \sum_{k''} w_{k''} \rho_1^{(k'')} \otimes \rho_2^{(k'')} \tag{19a}$$

then one has biorthogonality between the two groups of terms:

$$\forall k', \forall k'': \qquad \rho_i^{(k')} \rho_i^{(k'')} = 0 \qquad i = 1, 2. \tag{19b}$$

Before we prove the theorem, we first prove subsidiary results.

Lemma 1. *Let*

$$\rho_{12} = \sum_m w_m |\Psi^{(m)}\rangle_{12} \langle \Psi^{(m)}|_{12}$$

be an arbitrary pure-state mixture. Then, a pair of subsystem observables (A_1, A_2) are twins for ρ_{12} if and only if they are twins for all pure-state terms.

Proof. *Necessity* follows from the general result that all twins of ρ_{12} are also twins of all state vectors from the topological closure $\bar{\mathcal{R}}(\rho_{12})$ of the range of ρ_{12} (cf section 3, C1 in [1]). As is well known, the vectors $\{|\Psi^{(m)}\rangle_{12} : \forall m\}$ span the above-mentioned subspace.

Sufficiency is obvious. □

Lemma 2. *Let*

$$\rho_{12} = \sum_k w_k \rho_{12}^{(k)}$$

be an arbitrary mixture. The pair (A_1, A_2) are twin observables for ρ_{12} if and only if they are twin observables for all term states $\rho_{12}^{(k)}$.

Proof. This is immediately obtained from lemma 1 if one rewrites each term state as a pure-state mixture. □

Lemma 3. *An uncorrelated state $\rho_1 \otimes \rho_2$ has only trivial twins.*

Proof. This is an immediate consequence of the fact that the tensor factors of a nonzero uncorrelated vector, say $a \otimes b$, are unique up to an arbitrary nonzero complex number α, but if a is replaced by αa, b must be replaced by $(1/\alpha)b$.

If two observables are twins for an uncorrelated state, then

$$A_1 \rho_1 \otimes \rho_2 = \rho_1 \otimes A_2 \rho_2.$$

If $A_1\rho_1 = \alpha\rho_1$, then, applying the above remark to super-vectors, one has $\rho_2 = (1/\alpha)A_2\rho_2$. □

Proof of theorem 3. Now this immediately follows from lemmas 2 and 3. That is, the two groups of terms stated in the theorem make up the two terms in (3). □

Corollary 3. *Nontrivial twin events of a separable mixture (9) are necessarily strong twin events.*

Corollary 4. *If* (A_1, A_2) *are nontrivial twin observables for a separable mixture (9), they are strong twin observables (cf definition 3), and the mixture terms can be grouped into as many biorthogonal groups of terms as there are distinct characteristic values of* A_1 *in* $\mathcal{R}(\rho_1)$ *(generalization of (19a), (19b)).*

It is known that if a statistical operator and a Hermitian operator commute, then the corresponding state can be written as a mixture such that each term state has a definite value of the corresponding observable [10]. But, for the same statistical operator, there are also mixtures violating this.

To take an example, let us think of an unpolarized mixture of spin-half states: $\rho = (1/2)I$ (in the two-dimensional spin factor space). This statistical operator commutes with s_z; nevertheless, one can write down the mixture

$$\rho = (1/2)(|x,+\rangle\langle x,+| + |x,-\rangle\langle x,-|) = (1/2)I$$

in which the term states do not have a definite value of the z-component.

It is interesting that in the case of a separable mixture with a nontrivial twin observable, it is necessarily its term states that have the sharp detectable values of the corresponding observable.

7. States with maximally disordered subsystems

Now we turn to the example that is, for illustrative purposes, investigated in this study, i.e., to states (statistical operators) ρ in $\mathbb{C}^2 \otimes \mathbb{C}^2$. We say that ρ is an MDS state (one with maximally disordered subsystems or rather subsystem states) if $\rho_1 = (1/2)I_1$ and $\rho_2 = (1/2)I_2$. Horodecki and Horodecki have shown [11] that for every MDS state there exist unitary subsystem operators U_1 and U_2 such that

$$(U_1 \otimes U_2)\rho(U_1^\dagger \otimes U_2^\dagger) = (1/4)\left(I \otimes I + \sum_{i=1}^{3} t_i \sigma_i \otimes \sigma_i\right) \equiv T \tag{20}$$

where σ_i, $i = 1, 2, 3$, are the well known Pauli matrices σ_x, σ_y, and σ_z; and it is apparent from their position in the expression whether they relate to the first or the second spin-half particle.

Further, they have shown that the operator T is a statistical operator (a quantum state) if and only if the vector $\vec{t}$ from $\mathbb{R}_3$ whose components appear in (20) is not outside the *tetrahedron* determined as the set of all mixtures of the four pure *Bell states*:

$$|\psi_2^1\rangle \equiv (1/2)^{1/2}(|+\rangle|+\rangle \mp |-\rangle|-\rangle) \qquad |\psi_0^3\rangle \equiv (1/2)^{1/2}(|+\rangle|-\rangle \pm |-\rangle|+\rangle) \tag{21}$$

where $|+\rangle$ and $|-\rangle$ are the spin-up and the spin-down state vectors respectively.

It is straightforward to see that the three nonsinglet Bell states $|\psi_s\rangle$, $s = 1, 2, 3$, when written in the form (20), are given by $t_s = -1$, and that the other two components of $\vec{t}$ are equal to +1. The singlet state $|\psi_0\rangle$ is, in the form (20), determined by all three components of $\vec{t}$ being equal to -1.

It is also easy to see that for all mixtures one has

$$-1 \leqslant t_i \leqslant +1 \qquad i = 1, 2, 3.$$

This is a necessary but not a sufficient condition for T being a state. In other words, the tetrahedron is embedded in a cube, in which there are also nonphysical $\vec{t}$. In view of the LHS of (20), we call T that belong to the tetrahedron *generating MDS states*.

What we want to find out is: *which of the MDS states have nontrivial twins?* For those that do have, we want to find *the set of all nontrivial pairs of twins*.

It is sufficient to find the generating MDS states T with nontrivial twins, because the validity of

$$A_1 T = A_2 T$$

obviously implies

$$(U_1 A_1 U_1^\dagger)(U_1 U_2 T U_1^\dagger U_2^\dagger) = (U_2 A_2 U_2^\dagger)(U_1 U_2 T U_1^\dagger U_2^\dagger).$$

That is, if the generating MDS states have nontrivial twins, then the generated MDS states also have nontrivial twins, and they are immediately obtained.

As far as the pure generating MDS states (the Bell states) are concerned, the first-particle reduced statistical operator ρ_1 is equal to $(1/2)I_1$, and *all* nontrivial Hermitian operators A_1 commute with it; hence [3], they are twins. To evaluate the corresponding twin A_2, one has to read off the antilinear correlation operator U_a from (21), having in mind (11), and then utilize (13). For the best known Bell state, the singlet state $|\psi_0\rangle$, e.g. U_a takes $|+\rangle$ into $|-\rangle$, and $|-\rangle$ into $(-|+\rangle)$ (cf (21)). If

$$A_1 = \alpha_{++}|+\rangle\langle+| + \alpha_{--}|-\rangle\langle-| + \alpha_{+-}|+\rangle\langle-| + (\alpha_{+-})^*|-\rangle\langle+|$$
$$\alpha_{++}, \alpha_{--} \in \mathbb{R} \qquad \alpha_{+-} \in \mathbb{C}$$

then the twin A_2 has the form:

$$A_2 = \alpha_{--}|+\rangle\langle+| + \alpha_{++}|-\rangle\langle-| - \alpha_{+-}|+\rangle\langle-| - (\alpha_{+-})^*|-\rangle\langle+|.$$

Now we turn to the *mixtures of Bell states* in our search for nontrivial twins.

8. Mixtures of Bell states

Viewing statistical operators as super-vectors, and utilizing (redundantly, but for the sake of better overview) the ket notation for super-state vectors (i.e., Hilbert–Schmidt operators as normalized super-vectors), one can rewrite the generating vectors T given by (20) as a biorthogonal expansion with positive expansion coefficients:

$$|T\|T\|^{-1}\rangle_{12} = \left(1 + \sum_{i=1}^{3} t_i^2\right)^{-1/2} \Big(|(1/2)^{1/2} I\rangle_1 \otimes |(1/2)^{1/2} I\rangle_2 + \sum_{i=1}^{3} |t_i|\,|(1/2)^{1/2}\sigma_i\rangle_1 \otimes |\mathrm{sg}(t_i)(1/2)^{1/2}\sigma_i\rangle_2\Big) \qquad (22)$$

('sg' denotes the sign), i.e., as a (super-state-vector) *Hermitian Schmidt decomposition*.

One can read off (22) the following canonical entities of the super-state vector $|T\|T\|^{-1}\rangle_{12}$ (cf (10*a*), (10*b*) and (11)).

The first-subsystem reduced statistical super-operator $\hat{\rho}_1$ has the characteristic super-state vectors $\{|(1/2)^{1/2}I\rangle_1, |(1/2)^{1/2}\sigma_i\rangle_1 : i = 1, 2, 3\}$; the second-subsystem reduced statistical super-operator $\hat{\rho}_2$ has the characteristic state vectors $\{|(1/2)^{1/2}I\rangle_2, |\mathrm{sg}(t_i)(1/2)^{1/2}\sigma_i\rangle_2 : i = 1, 2, 3\}$; and the common spectrum of $\hat{\rho}_1$ and $\hat{\rho}_2$ is $\{R_0 \equiv (1 + \sum_{i=1}^{3} t_i^2)^{-1}, R_i \equiv R_0 t_i^2 : i = 1, 2, 3\}$. Finally, the antiunitary correlation super-operator $\hat{U}_a$ maps the enumerated characteristic state vectors of $\hat{\rho}_1$ into the correspondingly ordered ones of $\hat{\rho}_2$.

9. Nontrivial MDS twins

Every super-operator $\hat{A}_1$ that commutes with $\hat{\rho}_1$, i.e., for which every characteristic subspace of the latter is invariant (and no other super-operator), has a twin super-operator $\hat{A}_2$ [3]. But we are interested only in those pairs $(\hat{A}_1, \hat{A}_2)$ in which *both* super-operators are what may be called *multiplicative* ones, i.e., which have the form

$$\hat{A}_1\rho_{12} = A_1\rho_{12} \qquad \hat{A}_2\rho_{12} = A_2\rho_{12}$$

where A_p, $p = 1, 2$, are ordinary (subsystem) operators. It is easy to see that a multiplicative super-operator is *Hermitian* (in the Hilbert–Schmidt space of super-vectors) if the ordinary operator (in the usual sense) that determines it is also.

The basic result of the illustration expounded above is given in the following two theorems.

Theorem 5. *Mixed generating MDS states have nontrivial twins if and only if they are mixtures of two Bell states (binary mixtures).*

Theorem 6. *(A) Let us take a binary mixture of two Bell states both distinct from the singlet one, and let $T_i \equiv |\psi_i\rangle\langle\psi_i|$ (cf (21)) be the nonsinglet Bell state that does not participate in the mixture. Then the nontrivial twins are*

$$A_1 \equiv \alpha I_1 + \beta\sigma_i^{(1)} \qquad A_2 \equiv \alpha I_2 + \beta\sigma_i^{(2)} \qquad \alpha, \beta \in \mathbb{R} \qquad \beta \neq 0 \tag{23}$$

where the suffix on σ_i refers to the corresponding tensor factor space.

(B) In the case of a binary mixture of the singlet state with another Bell state, say $T_i \equiv |\psi_i\rangle\langle\psi_i|$ (cf (21)), the twins are

$$A_1 \equiv \alpha I_1 + \beta\sigma_i^{(1)} \qquad A_2 \equiv \alpha I_2 - \beta\sigma_i^{(2)} \qquad \alpha, \beta \in \mathbb{R} \qquad \beta \neq 0. \tag{24}$$

Proof of the two theorems and of some subsidiary results is given in the appendix. The proof of theorem 6 that is given first in the appendix is only of *methodological significance*: it illustrates a method for evaluating nontrivial twins. In our case of binary mixtures $T^{(2)}$, another method gives a simpler evaluation. It is given at the end of the appendix.

It is known that any Bell state can be converted into any other one by local unitary transformation [6, 12]. Hence, to prove the existence of nontrivial twins it would have sufficed to take mixtures of one pair of Bell states. Theorem 6 is, nevertheless, more elaborate, because the explicit form of the twins depends on which Bell states are involved.

It is known that all binary mixtures of Bell states are nonseparable except those with equal weights. The latter, as is easily seen, are examples of theorem 4; e.g., as one can easily ascertain making use of (21), one has

$$(1/2)((|+\rangle\langle+| \otimes |+\rangle\langle+|) + (|-\rangle\langle-| \otimes |-\rangle\langle-|)) = (1/2)(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|). \tag{25}$$

The nonseparable binary Bell state mixtures are distillable even in the single-copy case [13]. Unfortunately, there is no simple relation between the existence of nontrivial twins (being investigated) and distillability, as can be seen from the fact that rank-four mixtures are also distillable (if and only if one of the weights is larger than 1/2), and they do not have nontrivial twins.

In conclusion, I would like to point out that the entangled pure-state case [3, 4] is a well explored illustration of the fact that nontrivial twins can exist on account of *entanglement*. The nonseparable binary Bell state mixtures provide another simple illustration of this fact. One should keep it in mind that, as was seen in lemma 3, uncorrelated bipartite states do not have nontrivial twins. Separable states can have nontrivial twins if and only if biorthogonal grouping of the terms is possible (cf theorem 4). Unfortunately, for the time being, we do not have a necessary and sufficient condition for the existence of nontrivial twins on account of entanglement (except in the pure-state case), let alone a way of generating all of them for a given composite-system mixed state (except in the pure-state case).

Last, but not least, a relation between the reported twin investigation (see [3], [4], and [1], in addition to this paper) and the mainstream research on entanglement (take the cited Bennett *et al* articles, the article of Vedral *et al* and the cited Horodecki family articles as examples) is still lacking. But I believe that there is a connection. Further research will, one hopes, uncover it.

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Appendix

Since we are going to prove the theorems making use of (22), first we must be able to recognize the binary mixtures $T^{(2)}$ on the Horodecki tetrahedron.

Proposition A.1. *One has a binary mixture* $T^{(2)}$ *if and only if precisely one of the three values of* $|t_i|$ *in (22) equals* 1.

(A) If $t_i = +1$, $|t_{i+1}|, |t_{i+2}| < 1$ *(where the three values* $\{1, 2, 3\}$ *of i are meant cyclically), then the mixture is of two Bell states both distinct from the singlet state. If* T_i *is the nonsinglet Bell state that does not participate in the mixture, one has* $t_{i+2} = -t_{i+1}$. *Finally, the binary mixture* $T^{(2)}$ *in question is*

$$T^{(2)} = [(1 - t_{i+1})/2]T_{i+1} + [(1 - t_{i+2})/2]T_{i+2}. \tag{A.1}$$

(B) If $t_i = -1$, $|t_{i+1}|, |t_{i+2}| < 1$ *(in the cyclic sense), then one deals with a mixture of two states: the singlet state and another Bell state* T_i. *One has* $t_{i+1} = t_{i+2}$, *and the binary mixture* $T^{(2)}$ *in question is*

$$T^{(2)} = [(1 + t_{i+1})/2]T_i + [(1 - t_{i+1})/2]T_0. \tag{A.2}$$

Both in case (A) and in case (B), t_{i+1} can be any number in the interval $-1 \leqslant t_{i+1} \leqslant +1$; equivalently, one can have any point on the corresponding border of the Horodecki tetrahedron (the vertices excluded).

For the proof, a few subsidiary results are required.

Lemma A.1. *If among the four numbers* $\{1, |t_i| : i = 1, 2, 3\}$ *appearing in the form (22) of the generating MDS state T there is one distinct from the rest, then T has no nontrivial twins.*

Proof. As clearly follows from the spectrum of $\hat{\rho}_1$ given above, the above-mentioned 'one number distinct from the rest' corresponds to a nondegenerate characteristic value. Assuming that A_1 is a twin, it is a multiplicative super-operator reducing in each characteristic subspace of $\hat{\rho}_1$. (This is equivalent to commutation with $\hat{\rho}_1$.)

(a) Let us take the case where $|t_i| < 1$, $i = 1, 2, 3$. Then the first characteristic value of $\hat{\rho}_1$ is nondegenerate, and the corresponding characteristic super-state vector has to be invariant (up to a constant):

$$A_1(1/2)^{1/2}I_1 = \alpha(1/2)^{1/2}I_1$$

i.e., $A_1 = \alpha$, and the twin is trivial.

(b) Let $|t_i|$ for some value of i be distinct from the other three numbers. Then the corresponding characteristic super-state vector $\sigma_i(1/2)^{1/2}$ must be invariant (up to a constant):

$$A_1\sigma_i(1/2)^{1/2} = \alpha\sigma_i(1/2)^{1/2}$$

which, upon multiplication with σ_i from the right, implies $A_1 = \alpha$ again. □

Corollary A.1. *If a generating MDS state T has nontrivial twins, then for at least one value of i, $|t_i| = 1$.*

Proof. This is obvious from lemma A.1. □

Lemma A.2. *Expressing a generating MDS state T written in the form (22) in terms of the statistical weights with respect to the Bell states $\{T_k \equiv |\psi_k\rangle\langle\psi_k| : k = 0, 1, \ldots, 3\}$ (cf (6)), one has*

$$T = \sum_{k=0}^{3} w_k T_k = (1/4)[I \otimes I + (-w_1 + w_2 + w_3 - w_0)\sigma_1 \otimes \sigma_1 + (w_1 - w_2 + w_3 - w_0)\sigma_2 \otimes \sigma_2 + (w_1 + w_2 - w_3 - w_0)\sigma_3 \otimes \sigma_3] \tag{A.3}$$

where

$$\forall k: \qquad w_k \in [0, 1] \qquad k = 0, 1, 2, 3 \qquad \sum_{k=0}^{3} w_k = 1.$$

Proof. This is straightforward, substituting the Bell states in (22) (cf (21) and beneath it). □

Lemma A.3. *If one has $|t_i| = 1$, $i = 1, 2, 3$, for a generating MDS state T in the form (22), then it is a Bell state.*

Proof. Each t_i has two sign possibilities; altogether there are $2^3 = 8$ possibilities. A straightforward analysis of each of these, taking into account lemma A.2 and $\sum_{k=0}^{3} w_k = 1$, shows that four possibilities do not give states. These are: $\{\mathrm{sg}(t_i) = + : i = 1, 2, 3\}$, $\{+ - -\}$, $\{- + -\}$, and $\{- - +\}$. The remaining four sign possibilities give the four Bell states:

$$\{- + +\}: T_1 \qquad \{+ - +\}: T_2 \qquad \{+ + -\}: T_3 \qquad \{- - -\}: T_0.$$

□

Proof of claim (A) in proposition A.1. Since it is clear from (A.3) that the t_i as functions of w_k are symmetric (in the sense of the cycle $\{1, 2, 3\}$), it is sufficient to take $i = 1$. Then

$$-w_1 + w_2 + w_3 - w_0 = 1 \qquad \text{and} \qquad \sum_{k=0}^{3} w_k = 1.$$

This gives $w_2 + w_3 = 1$, $w_1 = w_0 = 0$, and $t_2 = w_3 - w_2 = -t_3$. Hence, $w_2 = (1 - t_2)/2$ and $w_3 = (1 + t_2)/2$ as claimed. Since $0 < w_1, w_0 < 1$, the claimed intervals for t_2 and t_3 follow. □

Proof of claim (B) of the proposition. This runs in full analogy with the proof for case (A). □

Proof of the main claim of the proposition. It is easy to see that the proofs of claims (A) and (B) of the proposition carry over to the case where $|t_{i+1}|$ or $|t_{i+2}|$ equals one. Hence, one cannot have $|t_i| = 1$ for precisely two values of i. If this is the case for one value, then either it is so for all three values, and one has a pure Bell state, or it is so for precisely one value of i, and then we have a binary mixture. □

Proof of theorem 6. We now assume that for one value of i, $|t_i| = 1$, and that the other two components of $\vec{t}$ in (22) have moduli less than one. Then it is sufficient and necessary for an observable A_1 that defines a super-operator $\hat{A}_1$ by multiplication (we write this as $\hat{A}_1 \equiv (A_1\bullet)$) to have a super-operator twin A_2 (that is not necessarily multiplicative like $\hat{A}_1$) to reduce in the two-dimensional super-vector subspace spanned by I_1 and $\sigma_i^{(1)}$. If we write $A_1 = \alpha I_1 + \sum_{j=1}^{3} \beta_j \sigma_j^{(1)}$ ($\alpha, \beta_j \in \mathbb{R}$), and multiply with this from the left by $\sigma_i^{(1)}$, it turns out that the condition amounts to $\beta_j = 0$, $j \neq i$. A symmetrical argument gives the symmetrical result. Thus the multiplicative super-operators defined by A_1 and, separately, by A_2 have super-operator twins if and only if they are of the form

$$A_1 = \alpha I_1 + \beta\sigma_i^{(1)} \qquad A_2 = \gamma I_2 + \delta\sigma_i^{(2)} \tag{A.4}$$

where $\alpha, \beta, \gamma, \delta \in \mathbb{R}$.

The above-mentioned operators are twins of each other if and only if

$$(A_2\bullet) = \hat{U}_a (A_1\bullet)\hat{U}_a^{-1}. \tag{A.5}$$

Now we find the necessary and sufficient conditions for which (A.5) is valid for the operators given by (A.4). Since both sides of (A.5) are linear operators, we apply them to the basis of super-vectors $\{I_2, \sigma_i^{(2)} : i = 1, 2, 3\}$:

$$(A_2\bullet)I_2 = \gamma I_2 + \delta\sigma_i^{(2)}$$
$$(\hat{U}_a(A_1\bullet)\hat{U}_a^{-1})I_2 = \hat{U}_a(\alpha I_1 + \beta\sigma_i^{(1)}) = \alpha I_2 + \mathrm{sg}(t_i)\beta\sigma_i^{(2)}.$$

Thus, we obtain the condition

$$\gamma = \alpha \qquad \delta = \mathrm{sg}(t_i)\beta.$$

Utilizing the well known relation

$$\sigma_i\sigma_j = \delta_{ij} I + \sum_{m=1}^{3} \mathrm{i}\epsilon_{ijm}\sigma_m$$

we, further, have

$$\begin{aligned}
(A_2\bullet)\sigma_j^{(2)} &= (\gamma I_2 + \delta\sigma_i^{(2)})\sigma_j^{(2)} = \gamma\sigma_j^{(2)} + \delta\left(\delta_{ij} I_2 + \sum_m \mathrm{i}\epsilon_{ijm}\sigma_m^{(2)}\right)\\
(\hat{U}_a(A_1\bullet)\hat{U}_a^{-1})\sigma_j^{(2)} &= \mathrm{sg}(t_j)\hat{U}_a(\alpha I_1 + \beta\sigma_i^{(1)})\sigma_j^{(1)}\\
&= \mathrm{sg}(t_j)\hat{U}_a\left(\alpha\sigma_j^{(1)} + \beta\left(\delta_{ij} I_1 + \sum_m \mathrm{i}\epsilon_{ijm}\sigma_m^{(1)}\right)\right)\\
&= \mathrm{sg}(t_j)\left(\alpha\,\mathrm{sg}(t_j)\sigma_j^{(2)} + \beta\left(\delta_{ij} I_2 - \sum_m \mathrm{i}\epsilon_{ijm}\,\mathrm{sg}(t_m)\sigma_m^{(2)}\right)\right).
\end{aligned}$$

For $i = j$ we obtain the condition $\gamma = \alpha$, and $\delta = \mathrm{sg}(t_i)\beta$, and, for $j \neq i$, in addition, $\delta = -\mathrm{sg}(t_j)\,\mathrm{sg}(t_m)\beta$. Since $i \neq m \neq j$, we know from the proposition that, irrespective of $\mathrm{sg}(t_i)$, one has $-\mathrm{sg}(t_j)\,\mathrm{sg}(t_m) = \mathrm{sg}(t_i)$. Hence, we actually obtain the condition expressed by (23) and (24). □

The claim in theorem 5 that binary mixtures $T^{(2)}$ have nontrivial twins is an immediate consequence of theorem 6.

The above-mentioned second, simpler, proof goes as follows: according to lemma 1, a pair of opposite-subsystem observables (A_1, A_2) are twins for a composite-system mixture if and only if they are simultaneously twins for each of the pure term states.

Utilizing (13), it is straightforward to evaluate the twins in the operator basis consisting of the four super-vectors $|\pm\rangle\langle\pm|$. But for comparison with the results (23) and (24) obtained by the Hermitian Schmidt decomposition method, we do this in a slightly more difficult way using the form (22) for the Bell states (see their description beneath (22)).

We can read off the antiunitary correlation super-operator $\hat{U}_a$ from the above-mentioned form (22) of the Bell state. As was stated before, every first-subsystem observable $A_1 \equiv \alpha I_1 + \sum_{i=1}^{3} \beta_i \sigma_i^{(1)}$ ($\alpha, \beta_i \in \mathbb{R}, i = 1, 2, 3$) is a twin. The corresponding second-subsystem twins for the Bell states are

$$
\begin{aligned}
T_1&: \qquad A_2 \equiv \alpha I_2 - \beta_1 \sigma_1^{(2)} + \beta_2 \sigma_2^{(2)} + \beta_3 \sigma_3^{(2)} \\
T_2&: \qquad A_2 \equiv \alpha I_2 + \beta_1 \sigma_1^{(2)} - \beta_2 \sigma_2^{(2)} + \beta_3 \sigma_3^{(2)} \\
T_3&: \qquad A_2 \equiv \alpha I_2 + \beta_1 \sigma_1^{(2)} + \beta_2 \sigma_2^{(2)} - \beta_3 \sigma_3^{(2)} \\
T_0&: \qquad A_2 \equiv \alpha I_2 - \beta_1 \sigma_1^{(2)} - \beta_2 \sigma_2^{(2)} - \beta_3 \sigma_3^{(2)}.
\end{aligned}
$$

Now, in view of the position of the minus sign in A_2, evidently, utilizing $m \neq i \neq j \neq m$ ($i, j, m \in \{1, 2, 3\}$) and $0 < w < 1$, the simultaneous twins are

$$
\begin{aligned}
wT_j + (1-w)T_m&: \qquad A_2 \equiv \alpha + \beta_i \sigma_i \\
wT_0 + (1-w)T_i&: \qquad A_2 \equiv \alpha - \beta_i \sigma_i
\end{aligned}
$$

and A_2 is, of course, the twin of $A_1 \equiv \alpha + \beta_i \sigma_i$.

In this way, proof of (23) and (24) is obtained.

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