Fidelity and concurrence of conjugated states

Armin Uhlmann
Institut für Theoretische Physik, Universität Leipzig, D-04109 Leipzig, Germany
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We prove some properties of fidelity (transition probability) and concurrence, the latter defined by a straightforward extension of Wootters' notation. Choose a conjugation and consider the dependence of fidelity or of concurrence on conjugated pairs of density operator. These functions turn out to be concave or convex roofs. Optimal decompositions are constructed. Some applications to two and tripartite systems illustrate the general theorems.

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I. INTRODUCTION

In physics antilinearity is well known from symmetries with time reversal operations [1], from second quantization, and from representation theory of groups and algebras. Quantum information theory offers several interesting applications of antilinearity. In the present paper we are concerned with one of them. Antilinear operators are intrinsically nonlocal: One cannot tensor them consistently with the identity operator. They do not share the privilege of linear operators [2] to allow execution in one part of a bipartite system while "doing nothing" in the other one. It seems, therefore, quite natural to use antilinear operators to describe or to estimate effects of entanglement. Indeed, Hill and Wootters in Ref. [3] and Wootters in Ref. [4] used a particular conjugation, the *Hill-Wootters conjugation*, in order to get an explicit expression for the *entanglement of formation* for two qubits. Their papers are the very starting point for the present contribution. I tried to distill a general method out of their proofs, and to construct explicitly the relevant optimal decompositions. The entanglement of formation concept is due to Bennett *et al.* [5]. Also a peculiar basis, the *magic basis*, with which one can define the Hill-Wootters conjugation, is already in that important paper.

In the two-qubit case the entanglement of formation is a function of just one other quantity, called (pre)concurrence, [4] and the same optimal decomposition of a state into pure ones can be used to calculate its entanglement of formation and its concurrence. In this form the statement becomes wrong for general states of a bipartite system different from the 2×2 case. But for density operators of rank two similar results seem not out of range.

However, concurrence seems to be an interesting quantity in its own. It can be defined in higher-dimensional Hilbert spaces and with respect to any conjugation Θ by an explicit expression (Sec. II) which will be called Θ concurrence. It is a convex function on the state space (Sec. III), and it is a roof (see Sec. V). Optimal decompositions can be obtained (Sec. IV) in a constructive manner, adding some news even for the two-qubit case. Generally, the length of an optimal decompositions will be the smallest power of two which exceeds the dimension of the Hilbert space.

The idea, pointing to the definition of Θ concurrences, can be extended to another interesting quantity, to the fidelity, the square root of the transition probability [6]. Θ fidelity as defined in Sec. II, turns out to be a concave roof. Optimal decompositions can be gained similarly.

The main proofs are in Secs. III and IV. Section V is devoted to the roof concept [7], an interesting tool if combined with convexity or concavity. The last section contains some applications, mainly of Θ concurrences. There are conjugations in multipartite systems such that a nonzero Θ concurrence indicates inseparability. It is illustrated for bipartite (example 1) and for the three-qubit systems (example 3). In a $2\times n$ bipartite system there is the possibility to bound entanglement of formation from below by the aid of Θ concurrences (example 2). After extending the method slightly (theorem 5) to a larger class of antilinear operators, example 4 treats Θ fidelity and concurrence on some two-dimensional subspaces of the two-qubit system. Though the result is essentially known for the concurrence [3] it explains a part of the method.

Now I shortly call attention to some notations and rules, connected with antilinearity, to prepare what follows below. An *antilinear* operator ϑ acting on an Hilbert space $\mathcal{H}$ satisfies by definition

$$\vartheta(a_1\psi_1+a_2\psi_2)=a_1^*\psi_1+a_2^*\psi_2 .$$

If ψ is an eigenvector of ϑ with eigenvalue λ, $\epsilon\psi$ is an eigenvector with eigenvalue $\epsilon^{-2}\lambda$ for all unimodular numbers ϵ. The fact that the eigenvalues of an antilinear operator fill some circles in the complex plain will be used in the estimations of Sec. III. The product of two antilinear operators becomes linear, the product of an of antilinear operator and a linear one remains antilinear. The adjoint (or Hermitian adjoint) $\vartheta^\dagger$ of an antilinear operator ϑ is determined by the relation

$$\langle\psi,\vartheta^\dagger\varphi\rangle=\langle\varphi,\vartheta\psi\rangle$$

for all $\psi,\varphi\in\mathcal{H}$. Notice $(\vartheta^\dagger)^\dagger=\vartheta$. The standard rule $(AB)^\dagger=B^\dagger A^\dagger$ for linear operators remains valid if one or both operators are replaced by antilinear ones. In particular, with a complex number a and antilinear ϑ one gets $(a\vartheta)^\dagger=\vartheta^\dagger a^*=a\vartheta^\dagger$, i.e., taking the adjoint is a linear procedure for antilinear operators. It follows that the set of operators which are antilinearly Hermitian (antilinearly self-adjoint), $\vartheta=\vartheta^\dagger$, is a linear space of dimension $d(d+1)/2$ if $\dim\mathcal{H}=d$. Indeed, ϑ is antilinearly Hermitian iff $\langle\psi,\vartheta\varphi\rangle$ is symmetric. With respect to a basis the condition restricts the off-diagonal entries only. Complex diagonal entries are allowed.

One calls ϑ antilinearly unitary or simply antiunitary if $\vartheta^\dagger = \vartheta^{-1}$. Basic knowledge about antiunitary operators is due to Wigner [1]. A conjugation Θ is an antiunitary satisfying $\Theta^2 = \mathbf{1}$. Writing $\Theta = \Theta^{-1} = \Theta^\dagger$ shows the hermiticity (self-adjointness) of conjugations. Well studied examples are time reversal operators [8] for Bose particles and for quantum systems with total integer angular momentum .

A conjugation Θ distinguishes in $\mathcal{H}$ a real subspace $\mathcal{H}_\Theta$, consisting of all Θ-invariant vectors, i.e., of all eigenvectors of Θ with eigenvalue 1. No real subspace in $\mathcal{H}$ is properly larger than $\mathcal{H}_\Theta$. Due to Hermiticity, $\Theta\psi = \psi$ and $\Theta\varphi = \varphi$ result in

$$\langle \psi, \varphi \rangle = \langle \varphi, \psi \rangle$$

so that the scalar product becomes real if restricted to $\mathcal{H}_\Theta$. In other words, $\mathcal{H}_\Theta$ is not only a real subspace, it is a *real Hilbert* subspace. On the other hand, Θ can be gained as complex conjugation in *every* basis contained in $\mathcal{H}_\Theta$. This establishes a one-to-one correspondence between maximal real Hilbert subspaces and conjugations.

In a one-qubit space, i.e., $\dim \mathcal{H} = 2$, a conjugation induces a reflection of the Bloch sphere at a certain plane through its center. Selecting the 1-2 plane, the plane perpendicular to the three-axis, as invariant plane, the effect of the conjugation to the Hermitian operator

$$\varrho = \tfrac{1}{2}(x_0 \mathbf{1} + x_1 \sigma_1 + x_2 \sigma_2 + x_3 \sigma_3), \tag{1}$$

that is, $\varrho \mapsto \tilde{\varrho} \equiv \Theta \varrho \Theta$, reads

$$\tilde{\varrho} = \tfrac{1}{2}(x_0 \mathbf{1} + x_1 \sigma_1 + x_2 \sigma_2 - x_3 \sigma_3). \tag{2}$$

Given a conjugation and a state vector ψ we shall consider the absolute value of the transition amplitude between ψ and $\Theta\psi$ or, what is the same, the square root of the transition probability between them. The quantity in question $|\langle \psi, \Theta\psi \rangle|$ is well defined for pure states. The problem addressed in the paper is to extend it to all states in a canonical way. In other words, we look for functions on the state space which are completely determined by their pure state behavior. This can be done by relying on the convex nature of the set of all density operators (states) which reflects the process of performing Gibbsian mixtures, i.e., of convex sums. There is one and only one largest convex function coinciding at pure states with $|\langle \psi, \Theta\psi \rangle|$, and, following Wootters, I call it Θ concurrence. And there is exactly one smallest concave function within all functions which are concave extensions from the chosen values for pure states to all density operators. That function I call Θ fidelity.

II. FIDELITY AND CONCURRENCE

Let ϱ and ω be two density operators in an Hilbert space $\mathcal{H}$. Their transition probability is denoted by $P(\varrho, \omega)$, their fidelity, the square root of the transition probability, is called $F(\varrho, \omega)$. It holds

$$\sqrt{P(\varrho,\omega)} = F(\varrho,\omega) = \mathrm{tr}(\sqrt{\omega}\varrho\sqrt{\omega})^{1/2}. \tag{3}$$

Let $\mathcal{H}^a$ be an ancillary Hilbert space. For any two vectors, $\varphi, \psi \in \mathcal{H} \otimes \mathcal{H}^a$, which reduce to ϱ and ω,

$$\varrho = \mathrm{Tr}_a |\varphi\rangle\langle\varphi|, \quad \omega = \mathrm{Tr}_a |\psi\rangle\langle\psi|,$$

the transition amplitude is bounded from above by the fidelity $|\langle \varphi, \psi \rangle| \leqslant F(\varrho, \omega)$. Indeed, $F(\varrho, \omega)$ is the least number which fulfills this condition. Equivalently, as $F^2 = P$, a suitably chosen von Neumann measurement in an ancillary system can cause a transition $\varrho \mapsto \omega$ with probability $P(\varrho, \omega)$. A larger transition probability, however, is not possible [6]. The joined concavity of the fidelity can be seen from

$$F(\varrho,\omega) = \inf_X \tfrac{1}{2}[\mathrm{tr}(X\varrho) + \mathrm{tr}(X^{-1}\omega)], \tag{4}$$

where X runs through all positive and invertible operators X. A proof for finite-dimensional Hilbert spaces is as follows: Abbreviate by a and b the traces over $X\varrho$ and $X^{-1}\omega$, respectively. From Ref. [9] one knows $F^2 \leqslant ab$. But $2\sqrt{ab} \leqslant a + b$, and the right hand side of Eq. (4) cannot be smaller than the left one. If the density operators are invertible then there is a unique positive solution X of

$$X\varrho X = \omega, \quad X = \varrho^{-1/2}(\varrho^{1/2}\omega\varrho^{1/2})\varrho^{-1/2}.$$

With this solution we get $a = b$ and $a = F$, and Eq. (4) is saturated. Now we use continuity to extend the proof to all pairs of density operators. See also Ref. [10].

It is useful to extend Eqs. (3),(4), and similar ones to all positive operators with finite trace. The simple scaling properties of P, F, and related quantities make this is an easy task. Of course, the physical interpretation of P as a probability is bound to normalized density operators.

Let Θ be a conjugation in an Hilbert space $\mathcal{H}$ and abbreviate $\tilde{\varrho} \coloneqq \Theta\varrho\Theta$. It is evident from Eq. (4) that

$$F_\Theta(\varrho) \coloneqq F(\varrho, \tilde{\varrho}) \tag{5}$$

is concave in ϱ [11]. Equation (5) will be called Θ fidelity of ϱ.

In order to introduce the (pre)concurrence [5,4] we need the ordered singular numbers $\lambda_1 \geqslant \lambda_2 \geqslant \cdots$ of $\sqrt{\varrho}\sqrt{\omega}$, that is,

$$\{\lambda_1 \geqslant \lambda_2 \geqslant \cdots\} = \text{spectrum of} \quad (\sqrt{\varrho}\,\omega\sqrt{\varrho})^{1/2}. \tag{6}$$

Having in mind Wootters' explicit expression for the entanglement of formation it is tempting to define for any two density operators (whether normalized or not) the function

$$C(\varrho,\omega) \coloneqq \max\left\{0, \lambda_1 - \sum_{j>1} \lambda_j\right\} \tag{7}$$

and to call it concurrence of ϱ and ω.

A useful relation can be obtained if the rank of $\varrho\omega$ does not exceed two. Adding $P = F^2$ to C^2 the cross terms in the two nonvanishing eigenvalues cancel. But the sum of the squared eigenvalues (6) is equal to the trace of $\varrho\omega$. Hence

$$C(\varrho,\omega)^2+F(\varrho,\omega)^2=2\,\mathrm{Tr}(\varrho\omega)\quad \text{if rank}\quad(\varrho\omega)\leqslant 2. \tag{8}$$

Finally, given a conjugation Θ, we call Θ congruence of ϱ the concurrence between ϱ and its conjugate $\tilde{\varrho}$,

$$C_\Theta(\varrho):=C(\varrho,\tilde{\varrho}),\quad \tilde{\varrho}=\Theta\varrho\Theta. \tag{9}$$

In contrast to the higher-dimensional cases it is not hard to get explicit expressions if $\dim\mathcal{H}=2$. With ϱ given by Eq. (1) and a conjugation acting as in Eq. (2) one obtains

$$F_\Theta(\varrho)=\sqrt{x_0^2-x_3^2},\quad C_\Theta(\varrho)=\sqrt{x_1^2+x_2^2}. \tag{10}$$

The next issue is to prove that F_Θ is a concave and C_Θ is a convex roof for every conjugation Θ in every finite dimensional Hilbert space. For the time being the finite dimensionality of the Hilbert space is essential due to some unexamined mathematical problems in the case of infinite dimensions. Thus, in all what follows, $\dim\mathcal{H}=d<\infty$.

III. PROPERTIES OF Θ FIDELITY AND Θ CONCURRENCE

In this section we derive some implications from and begin the proof of Theorem 1.

Theorem 1: Let Θ be a conjugation. Then

$$C_\Theta(\varrho)=\min\sum |\langle\phi_k|\Theta|\phi_k\rangle|,$$

$$F_\Theta(\varrho)=\max\sum |\langle\phi_k|\Theta|\phi_k\rangle|, \tag{11}$$

where the min and max has to run through all ensembles $\{\phi_1,\phi_2,\dots\}$ such that

$$\varrho=\sum |\phi_k\rangle\langle\phi_k| \tag{12}$$

is valid.

The proof of the theorem will terminate in the next section. Up to that point we consider (11) as a definition of its left-hand-sides, and we shall draw conclusions without using Eqs. (5) and (9) of the preceding section.

Consider first the case $\varrho=|\psi\rangle\langle\psi|$. Clearly, every decomposition (12) is gained by $\phi_k=a_k\psi$ with numbers a_k satisfying $\Sigma|a_k|^2=1$. Hence

$$C_\Theta(|\psi\rangle\langle\psi|)=F_\Theta(|\psi\rangle\langle\psi|)=|\langle\psi|\Theta|\psi\rangle|. \tag{13}$$

A simple consequence of Eq. (11) is homogeneity. For positive reals

$$C_\Theta(\mu\varrho)=\mu C_\Theta(\varrho),\quad F_\Theta(\mu\varrho)=\mu F_\Theta(\varrho),\quad \forall\mu\geqslant 0. \tag{14}$$

Being in finite dimension the minimum (maximum) in Eq. (11) will be attained by certain decompositions (12). They are called optimal decompositions.

Choosing optimal decompositions for $C_\Theta(\varrho)$ and $C_\Theta(\omega)$, their union is a decomposition for $C_\Theta(\varrho+\omega)$, though not necessarily an optimal one. Hence $C_\Theta(\varrho)+C_\Theta(\omega)$ is an upper bound for $C_\Theta(\varrho+\omega)$. Similar reasoning can be done for the Θ fidelity. Thus

$$C_\Theta(\varrho+\omega)\leqslant C_\Theta(\varrho)+C_\Theta(\omega),$$
$$F_\Theta(\varrho+\omega)\geqslant F_\Theta(\varrho)+F_\Theta(\omega) \tag{15}$$

showing subadditivity of Θ concurrence and superadditivity of Θ fidelity. Because of its homogeneity (14) we conclude that C_Θ is convex and F_Θ is concave.

Now we can go a step further, again without using arguments from the preceding section. Let Ω be the state space, i.e., the convex set of normalized density operators. If ϱ is in this set, a decomposition (12) can be rewritten as a convex combination

$$\varrho=\sum p_k\pi_k,\quad \pi_k=\frac{|\phi_k\rangle\langle\phi_k|}{\langle\phi_k|\phi_k\rangle}. \tag{16}$$

Assuming that our decomposition (16) is optimal for, say, the Θ concurrence, we can write

$$C_\Theta(\varrho)=\sum p_kC_\Theta(\pi_k).$$

We conclude the following [7]. Let C' be another convex function on Ω coinciding with C at the pure states. Then we have

$$C'(\varrho)\leqslant\sum p_kC'(\pi_k)=\sum p_kC_\Theta(\pi_k).$$

But for a an optimal decomposition which of the Θ concurrence the right hand sides coincides with $C_\Theta(\varrho)$. A similar proof is for F_Θ. It results in Theorem 2.

Theorem 2: C_Θ is the largest convex function and F_Θ is the smallest concave function on the state space coinciding with $|\langle\psi|\Theta|\psi\rangle|$ at the pure states.

To show that the right hand sides of Eq. (11) coincide with the definitions used in Sec. II, optimal decompositions will be gained in the next section.

IV. OPTIMAL DECOMPOSITIONS

In building optimal decompositions for our Θ fidelity and Θ concurrence the properties of antilinear operators play a decisive role. Fix a density operator ϱ and define an antilinear operator ϑ by

$$\vartheta\equiv\vartheta_\varrho:=\sqrt{\varrho}\Theta\sqrt{\varrho}. \tag{17}$$

Because $\Theta^\dagger=\Theta$, ϑ is antilinearly Hermitian. Hence

$$\langle\varphi,\vartheta\psi\rangle=\langle\psi,\vartheta\varphi\rangle.$$

Substituting $\varphi=\vartheta\psi$ proves all the expectation values of ϑ^2 real and not negative. Thus, ϑ^2 is a linear positive operator and the same is with $\sqrt{\vartheta^2}$. Let us abbreviate $\tilde{\varrho}=\Theta\varrho\Theta$, so that ϑ^2 can be written $\sqrt{\varrho}\tilde{\varrho}\sqrt{\varrho}$. Remark, just to see what is going on, how the eigenvalues of the positive square root of ϑ^2 have been used in Sec. II to express F_Θ and C_Θ.

Our next aim is to prove the existence of a conjugation, Θ_0, depending on ϱ, with which we can polar decompose

$$\vartheta = \Theta_0 \sqrt{\vartheta^2} = \sqrt{\vartheta^2}\,\Theta_0, \quad \vartheta^2 = \sqrt{\varrho}\,\tilde{\varrho}\,\sqrt{\varrho}. \tag{18}$$

Let $\lambda^2, \lambda > 0$ be an eigenvalue of ϑ^2 and $\mathcal{H}^\lambda$ the Hilbert subspace of the corresponding eigenvectors. With ψ also $\vartheta\psi$ belongs to $\mathcal{H}^\lambda$. Define on $\mathcal{H}^\lambda$ the action $\Theta_0\psi := \lambda^{-1}\vartheta\psi$. On $\mathcal{H}^\lambda$ the operator Θ_0 is a conjugation which commutes with ϑ. If one eigenvalue of ϑ^2 is zero, Θ_0 should induce on $\mathcal{H}^0$ an arbitrarily chosen conjugation. Now $\mathcal{H}$ is decomposed as a direct orthogonal sum of Hilbert spaces of the form $\mathcal{H}^\lambda$ and Θ_0 is given as an operator on every one of them. But this defines Θ_0 uniquely as a conjugation on $\mathcal{H}$, and Eq. (18) is proved. Choosing in every $\mathcal{H}^\lambda$ a Θ_0-invariant basis, we get a common eigenbasis $\{\psi_1, \psi_2, \dots\}$, such that

$$\vartheta\psi_k = \sqrt{\vartheta^2}\,\psi_k = \lambda_k \psi_k, \quad \Theta_0 \psi_k = \psi_k \tag{19}$$

with ordered eigenvalues $\lambda_1, \geqslant \lambda_2, \geqslant \cdots$.

The vectors constituting an optimal decomposition will be obtained by the help of real Hadamard matrices. They can be inductively gained by

$$A_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad A_{2m} := \begin{pmatrix} A_m & A_m \\ A_m & -A_m \end{pmatrix} \tag{20}$$

for $m = 2,4,8, \dots$. Let us denote by a_{ki} the matrix elements of A_m. These entries are either 1 or -1. They fulfill

$$\sum_{k=1}^{m} a_{ki} a_{kj} = m\,\delta_{ij}, \quad a_{1j} = 1 \,\forall j. \tag{21}$$

The number m is adjusted to the dimension d of $\mathcal{H}$ by

$$m = 2^{n+1}, \quad 2^n < \dim \mathcal{H} \leqslant 2^{n+1}. \tag{22}$$

With an arbitrary selection of d unimodular numbers (phase factors), $\epsilon_1, \epsilon_2, \dots$, we define with a basis (19) the vectors

$$\varphi_k = \sum_{i=1}^{d} a_{ki} \epsilon_i \psi_i, \quad k = 1,2, \dots, m. \tag{23}$$

By the help of Eqs. (23) and (21) it is straightforward to prove the following, essentially known identities

$$\sum_{k=1}^{m} |\varphi_k\rangle\langle\varphi_k| = m \sum_{i=1}^{d} |\psi_i\rangle\langle\psi_i| = m\mathbf{1} \langle\varphi_k|\vartheta|\varphi_k\rangle = \sum_{j=1}^{d} \epsilon_j^{-2}\lambda_j. \tag{24}$$

The remarkable deviation from most uses of Hadamard matrices is in the appearance of the phase factors produced by the antilinearity of ϑ. They provide sufficient flexibility in adjusting the expectation values of ϑ. By varying the ϵ_j in the second equation arbitrarily, the absolute values of the numbers $\langle\varphi_k|\vartheta|\varphi_k\rangle$ fill completely the following interval of real numbers:

$$\sum_{j=1}^{d} \lambda_j \geqslant \left| \sum_{j=1}^{d} \epsilon_j^{-2}\lambda_j \right| \geqslant \max\left\{ 0, \lambda_1 - \sum_{j=2}^{d} \lambda_j \right\}. \tag{25}$$

Proof: (a) The sum of the λ_j is an upper bound (triangle inequality) and it is reached with $\epsilon_j^{-2} = 1$ for all j. The simplest choice is $\epsilon_j = 1$ for all j. (b) If the λ_1 is not smaller than the sum of the remaining lambdas, a lower bound is $|\epsilon_1^{-2}\lambda_1 - x|$ where x is the maximum absolute value of $\epsilon_2^{-2}\lambda_2 + \epsilon_3^{-2}\lambda_3 + \cdots$. Hence we get the asserted lower bound. The bound is attained for $\epsilon^{-2} = 1$ and $\epsilon_j^{-1} = i$ for $j > 1$. (c) It remains to prove that if the assumption of (b) is not valid, the lower bound 0 should be reachable. In this case

$$\sum_{j=2}^{d} \lambda_j > \lambda_1 > \lambda_2 - \sum_{j=3}^{d} \lambda_j.$$

The first inequality is the assumption, the second follows because otherwise $\lambda_1 < \lambda_2$ in contradiction to the assumed ordering of the λ_k. We like to conclude the existence of a representation

$$\lambda_1 = \left| \sum_{j=2}^{d} \epsilon_j^{-2}\lambda_j \right|$$

as then the lower bound zero can be reached: We have to prove the same assertion as above, but now the length of the sum is $d-1$. Hence the proof is done if Eq. (25) is true for sums of length less than d. Starting with $d=2$, the proof terminates by induction to the length of the sum to be estimated.

Given $\lambda_1, \lambda_2, \dots$, we choose unimodular numbers $\epsilon_1, \epsilon_2, \dots$, saturating, respectively, the upper bound or the lower bound of Eq. (25). With this choice the vectors (23) are denoted by φ_k^+ (to refer to the upper bound) and by φ_k^- (to indicate the use of the lower bound), respectively. From the construction it follows that the insertion of

$$\phi_k^- = \sqrt{\varrho}\,\varphi_k^-, \quad \phi_k^+ = \sqrt{\varrho}\,\varphi_k^+, \quad k = 1, \dots, m \tag{26}$$

into Eq. (12) estimates Eq. (11) as follows:

$$C_\Theta \leqslant \max\left\{ 0, \lambda_1 - \sum_{j=2}^{d} \lambda_j \right\}, \quad F_\Theta \geqslant \sum \lambda_j.$$

These inequalities must be equalities. For the proof we use an arbitrary decomposition $\mathbf{1} = \Sigma |\chi_k\rangle\langle\chi_k|$ of the unity, insert $\phi_k = \sqrt{\varrho}\,\chi_k$ into Eq. (11), and convert the sum to be estimated with the help of Eq. (19) into

$$a \equiv \sum |\langle\phi_k, \Theta\,\phi_k\rangle| = \sum_k \sum_{j=1}^{d} |\lambda_j (\langle\chi_k, \psi_j\rangle)^2|.$$

At first we estimate concurrence by choosing the phases of ψ_j such that $\langle\chi_1, \psi_k\rangle$ becomes real and positive. We get

$$a = |\lambda_1 - b|, \quad b \equiv \sum_{j=2}^{d} \lambda_j \sum_k (\langle\phi_k, \psi_j\rangle)^2|$$

for the sum in question. If $|b|$ is larger than λ_1 we already obtained $a=0$ with $\phi_k=\phi^-$. In the other case $|b|$ cannot exceed $\lambda_2+\lambda_3+\cdots$, i.e., $a-|b|\leqslant C_\Theta$.

Concerning the Θ fidelity the Schwarz inequality will be applied to the positive Hermitian form $\langle\phi,\sqrt{\vartheta^2}\phi'\rangle$. Respecting Eqs. (18) and (19) one gets

$$|\langle\phi_k,\sqrt{\vartheta^2}\Theta_0\phi_k\rangle|\leqslant\langle\phi_k,\sqrt{\vartheta}\phi_k\rangle.$$

Therefore a cannot be larger than the trace of $\sqrt{\vartheta}$. The latter is equal to F_Θ and we arrive at $a\leqslant F_\Theta$. □

We have not only proved theorem 1 but also *Corollary 3*: Let $\dim\mathcal{H}=d$ and $2^n<d\leqslant 2^{n+1}$. For every ϱ there exist optimal decompositions for the Θ concurrence the length of which does not exceed 2^{n+1}. The same is true for the Θ fidelity.

Remarks. (a) Can the bounds for the optimal length become more stringent for certain dimensions of $\dim\mathcal{H}$. The construction above seems to deny it. But a proof is missing. (b) If $d=4=2\times 2$, then $n=2$ and there are optimal decompositions of maximal length four as shown by Wootters. See also [12] for the optimal length problem.

V. ROOFS

We now call attention to some peculiarities of convex or concave function on the state space which admit optimal decompositions. These functions are quite different from unitarily invariant ones such as, for instance, von Neumann entropy. The latter do not at all discriminate between pure states, they just estimate how strongly a state is mixed. Roofs, as defined below, and in particular convex or concave ones, draw all their information from their values at pure states. They try to interpolate between those values as linearly as possible. Let us see how it is achieved by two simple examples.

In two dimensions Θ fidelity and Θ concurrence are given by $\sqrt{1-x_3^2}$ and $\sqrt{x_1^2+x_2^2}$ on the unit ball $x_1^2+x_2^2+x_3^2\leqslant 1$, see Eq. (10). The first one remains constant on the planes $x_3=\text{const}$, the second one does so along the lines $x_1=c_1,\quad x_2=c_2$. The intersections of a plane or of a straight line with the unit ball are not only convex: The intersections can be gained as the convex hulls of the pure states they contain.

In turning to the general case we denote by Ω the convex set of all normalized density operators on a finite-dimensional Hilbert space and by Ω^{pure} the set of its extremal points, i.e., the set of pure density operators. A convex subset Ω_0 of Ω will be called a convex leaf of Ω if

$$\Omega_0=\text{convex hull of}\quad(\Omega_0\cap\Omega^{\text{pure}}).\tag{27}$$

Let $G=G(\varrho)$ be a function on Ω and Ω_0 a convex leaf of Ω. G is called convexly linear (or, equivalently, affine or flat) on Ω_0 if for all probability vectors $p_1,p_2,\ldots$ and for all choices of pure states

$$\pi_1,\pi_2,\ldots\in\Omega_0\cap\Omega^{\text{pure}}.\tag{28}$$

G satisfies the relation

$$G\Big(\sum p_j\pi_j\Big)=\sum p_jG(\pi_j).\tag{29}$$

It is not necessary to check condition (29) for all possible convex linear combinations in case G is either convex or concave:

Lemma R-1: Let G be convex or concave. If

$$\varrho=\sum q_j\pi_j,\quad q_k>0\tag{30}$$

is a decomposition of ϱ into pure density operators $\pi_1,\pi_2,\ldots$, and if

$$G(\varrho)=\sum q_jG(\pi_j)\tag{31}$$

is valid then G is convexly linear on the convex hull of $\pi_1,\pi_2,\ldots$.

Proof: Assume G is convex. Given ϱ, there is convexly linear function l satisfying $G\geqslant l$ on Ω, and $G(\varrho)=l(\varrho)$. Together with Eq. (31) we get

$$l(\varrho)=G(\varrho)=\sum q_jG(\pi_j)\geqslant\sum q_jl(\pi_j).$$

Because the right hand term is $l(\varrho)$, the $\geqslant$ symbol must be an equality sign. But $G\geqslant l$ now enforces $l(\pi_j)=G(\pi_j)$ for the pure states involved in Eq. (31). By the help of this equalities we estimate $G(\omega)$, $\omega=p_1\pi_1+\cdots$, by

$$l(\omega)\leqslant G(\omega)\leqslant\sum p_kG(\pi_k)=l(\omega)$$

and the inequality must be an equality. (The first inequality sign is due to $l\leqslant G$, the second due to the convexity of G.) This proves the lemma for convex G. Because $-G$ is convex if G is concave, the lemma remains true for concave functions. Another proof is in Ref. [13].

By definition, G is a roof if Ω can be covered by convex leaves such that G is convexly linear on every leaf of the covering. The covering is said to be a convex covering belonging to or compatible with G.

There is a simple geometric picture beyond. Assume a real number $g=g(\pi)$ is given for every pure state π. The idea is to think of a wall, made of straight lines starting from π and terminating at $g(\pi)\pi$. The demand is, to cover the state space Ω by a roof, founded upon the wall, which is as flat as possible. To satisfy the demand one joins every two points on the wall by a straight line, every three points by a triangle, and so on. If the dimension of the polyhedra becomes large enough, $(\dim\mathcal{H})^2$ in our case, the set of polyhedra covers Ω (an application of Caratheodory's theorem) and we stop. To get a roof we have to select a onefold covering of Ω from our huge set of polyhedra: There should be a function $\omega\rightarrow G(\omega)$ such that $x=G(\omega)$ whenever $x\omega$ is contained in one of the polyhedra of the selected covering. If it occurs, $G(\omega)\omega$ is a convex combination of the $g(\pi_j)\pi_j$ which generate the polyhedron. Taking the trace yields a representation

$$G(\omega)=\sum_{j=1}^{m} p_j g(\pi_j), \quad m \leqslant (\dim \mathcal{H})^2.$$

From the bewildering manifold of roofs we select the highest (or the lowest) one: Given ω we look for a polyhedron containing $x\omega$ with the largest (or with the smallest) possible real number x. Let us call this number $G^+(\omega)$, respectively, $G^-(\omega)$. There is such a polyedron if g is continuous, because then the set of all polyhedra based on a bounded number of edges is compact.

Some generalities can be abstracted from the construction above, see Refs. [14,7]. They are summarized in the following lemma.

Lemma R-2: Let $g=g(\pi)$ be a real and continuous function on the set of pure states.

(a) There is exactly one convex roof G^- and exactly one concave roof G^+ on Ω which coincides on $\Omega^{\rm pure}$ with g.

(b) G^+ is the smallest concave function and G^- is the largest convex function which coincides at the pure states with g.

(c) It is

$$G^+(\varrho)=\max\sum p_j g(\pi_j),$$

$$G^-(\varrho)=\min\sum p_j g(\pi_j),$$

where the variations have to run through all convex decompositions of ϱ with pure states.

Starting the discussion above from $g(\pi)=|\langle\psi,\Theta\psi\rangle|$, where $\pi=|\psi\rangle\langle\psi|$ and Θ is a conjugation, we arrive at $G^+=F_\Theta$ and $G^-=C_\Theta$. Within the pure states belonging to one of the optimal decompositions of the preceding section the values $g(\pi)$ remain constant. Hence G^+ and G^- are constant on the convex leaf they generate the following.

Corollary 4: The Θ concurrence (respectively the Θ fidelity) allows for a convex foliation such that C_Θ (respectively, F_Θ) is constant over every of its leaves.

As an immediate consequence, $\varrho\rightarrow f(C_\Theta(\varrho))$ and $\varrho\rightarrow f(F_\Theta(\varrho))$ are roofs over Ω for every function $f(x)$ defined on the unit interval. In general the roofs so obtained cease to be convex or concave. But there are some rules guaranteeing convexity (concavity) in some cases. To preserve convexity it suffices that f is convex and increasing. Concavity is guaranteed with f concave and decreasing [15].

Examples are C_Θ^s with real $1<s$ is a convex roof, F_Θ^s with $0<s<1$ is a concave roof. An important convex and increasing function, used by Hill and Wootters in Refs. [3] and [4] to get an expression for the entanglement of formation [5] reads

$$f_{HW}(x)=:s\left(\frac{1+\sqrt{1-x^2}}{2}\right)+s\left(\frac{1-\sqrt{1-x^2}}{2}\right), \qquad (32)$$

where $s(y)$ abbreviates $-y\ln y$. Thus

$$\varrho\mapsto f_{HW}(C_\Theta(\varrho)) \qquad (33)$$

is a convex roof for every conjugation in every Hilbert space. However, *only* if the Hilbert space is four dimensional, and Θ the Hill-Wootters conjugation, Eq. (33) is equal to the entanglement of formation. In bipartite $2\times 2n$ systems (33) can only be a lower bound to the entanglement of formation for appropriately chosen Θ (see the next section).

The following statements copy facts known in two-qubit systems to a more general frame. The maximum of F_Θ is one, and $F_\Theta=1$ is the equation of a convex leaf for F_Θ by lemma R-2. If $F_\Theta(\varrho)=1$ then $\Theta\varrho\Theta=\varrho$ by (5), and ϱ has a basis of Θ-invariant eigenvectors. The minimum of C_Θ is zero. The set of all states with vanishing Θ concurrence is a convex leaf with respect to C_Θ. If ϱ is Θ invariant, $\Theta\varrho\Theta=\varrho$, then $C_\Theta(\varrho)=0$ if and only if no eigenvalue of ϱ exceeds 1/2.

The entanglement of formation vanishes, as known from Ref. [5], exactly for separable, i.e., classically correlated states [16,17]. Separability in a two-qubit-system can equally well be characterized by the vanishing of C_Θ, Θ the Hill-Wootters conjugation. Again, just for two-qubits, $F_\Theta=1$ is the equation for the convex hull of the maximally entangled pure states.

VI. EXAMPLES

This section considers some possible applications of the general theorems. By looking at examples we ask whether Θ concurrences can be used to decide separability problems in bipartite and multipartite systems. In a two-qubit system a density operator is separable if and only if its concurrence vanishes. Could one suppose similar statements in a higher dimensional or in a multiqubit system? Certainly not with just one functional. But with sufficiently many it can work. Before treating the examples we have to return to a further issue in antilinearity.

All conjugations of an Hilbert space are unitarily equivalent. From Eq. (6) and the definitions of fidelity and concurrence one gets

$$F_{\Theta'}(\varrho)=F_\Theta(U\varrho U^\dagger), \quad C_{\Theta'}(\varrho)=C_\Theta(U\varrho U^\dagger)$$

with $\Theta'=U^\dagger\Theta U$ and every unitary operator U. However, in a bipartite or multipartite system,

$$\mathcal{H}=\mathcal{H}^a\otimes\mathcal{H}^b\otimes\otimes\mathcal{H}^c\cdots, \qquad (34)$$

one considers two conjugations equivalent iff there is a *local* unitary U such that $\Theta'=U^\dagger\Theta U$. Some of these equivalence classes consist of tensor products of antiunitary operators

$$\Theta=\theta_a\otimes\theta_b\otimes\cdots. \qquad (35)$$

To obtain a conjugation, the square of each factor must be a multiple of the appropriate identity, for example, $\theta_a^2=c_a\mathbf{1}^a$. According to Wigner there are only two possibilities $c_a=\pm 1$. Therefore, a factor in Eq. (35) is either a conjugation or it is an antiunitary satisfying $\theta^2=-\mathbf{1}$. The number of the latter cases must be even to obtain a conjugation by Eq. (35).

For the purpose of the present paper an antiunitary θ satisfying $\theta^2=-\mathbf{1}$ is called a skew conjugation. While skew conjugations are mostly discussed in connection with time reversal of fermions, we need them as building blocks for conjugations in multipartite quantum systems.

A skew conjugation fulfills $\theta^{-1}=-\theta^{\dagger}$ and

$$\langle \phi, \theta\phi' \rangle + \langle \phi', \theta\phi \rangle = 0. \tag{36}$$

All expectation values of a skew conjugation vanish. There is a consequence for vectors $\psi \in \mathcal{H}$ which are separable with respect to the first factor in Eq. (34), say $\psi = \phi^a \otimes \varphi$. If the first antiunitary, θ_a, is a skew conjugation, the expectation value $\langle \psi, \Theta\psi \rangle$ must vanish. In other words: Let Θ be a conjugation (35) and assume its first factor is a skew conjugation. If $\langle \psi, \Theta\psi \rangle$ is not zero, $|\psi\rangle\langle\psi|$ cannot be $\mathcal{H}^a$ separable.

A skew conjugation, θ, allows for a representation [1]

$$\theta\psi_{2j} = \psi_{2j-1}, \quad \theta\psi_{2j-1} = -\psi_{2j}, \tag{37}$$

$1 \le j \le n$, with a certain basis, $\psi_1, \psi_2, \dots$, called a θ basis. By Eq. (37) the Hilbert space decomposes into a direct sum of two-dimensional, θ invariant Hilbert subspaces. Of course, any basis of $\mathcal{H}$ can serve as a θ basis for a certain skew conjugation θ.

In one-qubit spaces there is, up to a phase, just one skew conjugation θ that may be defined by $|0\rangle \to i|1\rangle$, $|1\rangle \to -i|0\rangle$. (The imaginary unit in the definition is by convention.) On the state space it induces the well known spin flip. With that definition $\theta \otimes \theta$ is the Hill-Wootters conjugation of a two-qubit space.

Example 1: Consider in Eq. (34) a direct product $\mathcal{H} = \mathcal{H}^a \otimes \mathcal{H}^b$ of two even-dimensional Hilbert spaces. We distinguish a special class $\mathcal{F}$ of conjugations: $\Theta \in \mathcal{F}$ if the conjugation can be written as the product $\Theta = \theta^a \otimes \theta^b$ of two skew conjugations. Notice that, up to a phase, $\mathcal{F}$ consists of one conjugation in the two-qubit case, the Hill-Wootters one.

We have already seen from Eq. (36) that for this class $\langle \psi|\Theta|\psi \rangle = 0$ if ψ is a product vector. Thus $C_\Theta(\pi) = 0$ for every pure product state and for every $\Theta \in \mathcal{F}$. But, as seen at the end of the preceding section, the equation $C_\Theta(\varrho) = 0$ defines a convex leaf, i.e., C_Θ vanishes for all separable density operators. One may rephrase the statement by saying if ϱ is a state in a bipartite system and if we can find $\Theta \in \mathcal{F}$ such that $C_\Theta > 0$, then ϱ cannot be separable. We now complement the last statement: Let π be pure. If $C_\Theta(\pi) = 0$ is true for all $\Theta \in \mathcal{F}$ then π is a product state, i.e., separable.

For the proof we consider an arbitrary unit vector $\psi \in \mathcal{H}$ and assume $\dim \mathcal{H}^a = 2n \le \dim \mathcal{H}^b$. We use the Schmidt decomposition

$$\psi = \sum \alpha_j \phi_j^a \otimes \phi_j^b, \quad \alpha_1 \ge \alpha_2 \ge \cdots \tag{38}$$

to define a skew conjugations in the two parts of our bipartite system. θ_a is defined by requiring $\phi_1^a, \phi_2^a, \dots$, to be a θ_a basis. In $\mathcal{H}^b$ we complete, if necessary, the ϕ_j^b vectors to a basis which then is used as a the defining θ_b basis. After these preparations we consider $\Theta = \theta_a \otimes \theta_b$, a conjugation tailored for the vector (38). A straightforward calculation yields

$$\langle \psi|\Theta|\psi \rangle = 2\sum_{j=1}^{n} \alpha_{2j}\alpha_{2j-1}. \tag{39}$$

The sum on the right-hand-side can vanish only if all the Schmidt coefficients α_j vanish with the exception of the largest one. Hence ψ must be a product state.

Can we skip in the last statement the purity requirement? It seems unlikely with the exception of the two-qubit case. Thus we are faced with the problem to characterize the set of states with vanishing Θ concurrences for all conjugations from $\mathcal{F}$. Let us call the set of all these states Ω^c. As an intersection of convex leaves it is convex, but not necessarily a leaf. It contains all separable states. Moreover, a pure state is in Ω^c if and only if it is separable. But not all extremal points of Ω^c might be pure and, then, it will contain density operators which are not separable.

Example 2. We proceed with the setting of example 1 and require $\mathcal{H}^a$ to be two-dimensional. The requirement allows to bound the entanglement of formation from below for any even dimensional second factor $\mathcal{H}^b$ in the bipartite system. To do so we use Eq. (39) to establish

$$2\sqrt{\det \rho} = \sup_\Theta |\langle \psi, \Theta\psi \rangle|, \quad \Theta \in \mathcal{F}. \tag{40}$$

Here ρ denotes the partial trace of $|\psi\rangle\langle\psi|$ over the second factor $\mathcal{H}^b$. It then follows a lower bound for the entanglement of formation $E(\varrho)$.

$$E(\varrho) \ge \sup_\Theta f_{HW}(C_\Theta(\varrho)) = f_{HW}(\sup_\Theta C_\Theta(\varrho)), \tag{41}$$

where f_{HW} is explained by Eq. (32). The equality sign is due to the monotonicity of f_{HW}. The right-hand side of Eq. (41) is convex as a sup of convex functions of type (33). For pure states it coincides by Eq. (40) with the entanglement of formation. But the entanglement of formation is a convex roof by its definition, see Ref. [5] and point (c) of lemma R-2. Hence the left-hand side is the largest possible convex function with the described values for pure states.

Example 3. Now we try a similar procedure as in example 1 for a three-qubit-system. As already mentioned there is, after fixing a phase, only one skew conjugation, say θ, in a two-dimensional Hilbert space. Every conjugation in dimension two is of the form $U\theta$ with unitary U.

$\mathcal{H}$ in Eq. (34) is now the direct product of three 2-dimensional Hilbert spaces. Consider the conjugations

$$U\theta \otimes \theta \otimes \theta, \quad \theta \otimes U\theta \otimes \theta, \quad \theta \otimes \theta \otimes U\theta. \tag{42}$$

Let $\psi \in \mathcal{H}$ and Θ from this set. Then $\langle \psi|\Theta|\psi \rangle$ is zero if ψ is a product vector. A separable ϱ allows for a convex decomposition with product states by definition. For $C_\Theta = 0$ determines a convex leave, $C_\Theta(\varrho)$ has to vanish.

Turn now to the reverse and let be π a pure states with $C_\Theta(\pi) = 0$ for some conjugations listed in Eq. (42). The manifold of pure product states is eight-dimensional. We shall prove that eight equations $C_\Theta = 0$ with conjugations from Eq. (42) are sufficient to decide whether ψ is a product vector or not.

This goes as follows. Write ψ as a sum $|0\rangle|\varphi_0\rangle + |1\rangle|\varphi_1\rangle$ and start by the first set of conjugations listed in Eq. (42). We have to solve the equations

$$0 = \langle\psi|\psi\rangle = \sum \langle i|U\theta|j\rangle\langle\varphi_i|\tilde{\varphi}_j\rangle.$$

The tilde abbreviates the Hill-Wootters conjugation $\theta\otimes\theta$. With unitaries of the form $U|j\rangle = \epsilon_j|j\rangle$ we see that φ_k is orthogonal to $\tilde{\varphi}_k$. Hence φ_k is a product vector. To come to this conclusion, we need two diagonal unitaries. Next, with U equal to either σ_1 or σ_2, we see that φ_0 is orthogonal to $\tilde{\varphi}_1$. Because both are product vectors, either the first or the second one of their constituents has to be orthogonal one to another. Hence, after checking $C_\Theta = 0$ with 4 conjugations from our list, we arrive, up to a local unitary, at one of two possibilities:

$$|0\rangle|\phi\rangle|0\rangle + |1\rangle|\phi'\rangle|1\rangle, \quad |0\rangle|0\rangle|\phi\rangle + |1\rangle|1\rangle|\phi'\rangle.$$

Choosing now a conjugation from the second group of Eq. (42) yields $\langle\phi|U\theta|\phi'\rangle = 0$. We need just two of them to see that either $\phi = 0$ or $\phi' = 0$ has to take place, provided ϕ is located at the second position in the direct product. To cover also the case with ϕ in the third position, we need two conjugations from the third group.

Let π be a pure state of a three-qubit system. There are eight conjugations of the form (42) such that π is a product state if and only if $C_\theta(\pi) = 0$ is valid for all of them. It is tempting to ask whether one can prove similar statements for any multiqubit system. I believe the answer is affirmative, but I did not check it.

Last but not least we are going to cure a curious shortcoming of the treatment in example 1: It cannot be applied if one of the factors of the bipartite system is odd dimensional. The set $\mathcal{F}$ becomes empty. The same unsatisfactory event arises if no or only one factor of a multipartite system is even dimensional. Let us think, for example, the factor $\mathcal{H}^a$ is three-dimensional. To get an appropriate antilinear operator θ_a we split $\mathcal{H}^a$ into a direct sum of a two-dimensional and a one-dimensional Hilbert space. In the former we equal θ_a to a skew conjugation. In the latter we set θ_a to zero. We do not get an antiunitary operator, but an antilinear operator satisfying $\theta_a^\dagger = -\theta_a$. This relation suffices to guarantee Eq. (36). It seems natural, therefore, to allow in Eq. (35) the larger class of antilinear θ fulfilling $\theta^\dagger = \pm\theta$ as factors, and to require for the tensor product $\Theta^\dagger = \Theta$ only.

Returning to the bipartite system of example 1 we could consider the larger class of antilinear operators

$$\Theta = \theta_a\otimes\theta_b, \quad \theta_a^\dagger = -\theta_a, \quad \theta_b^\dagger = -\theta_b$$

so that Θ is antilinearly Hermitian and, nevertheless, $\langle\psi,\Theta\psi\rangle = 0$ for product vectors ψ. We arrive at the following general question: Do Θ fidelity (5) and Θ concurrence (9) remain concave respectively convex roofs for any antilinear self-adjoint Θ. Going through all the proofs one finds it essential that the antilinear operator $\vartheta := \sqrt{\varrho}\,\Theta\sqrt{\varrho}$ is antilinearly Hermitian. For that reason one proves by literally the same arguments.

Theorem 5. Let Θ be antilinear and self-adjoint, $\Theta = \Theta^\dagger$. Then

$$F_\Theta := F(\varrho, \Theta\varrho\Theta), \quad C_\Theta := C(\varrho, \Theta\varrho\Theta)$$

is a concave respectively a convex roof. Theorem 1 and Corollaries 3 and 4 remain valid for them.

Example 4. The final aim of the exercise is to determine fidelity and concurrence of certain conjugated states of rank two in in a two-qubit space. The reader should consider the example as representative for a lot of others which need more calculation effort.

Let $\mathcal{H}_2$ be a two-dimensional Hilbert space. The transition probability can be given by elementary algebraic operations [18]. For the present purpose an adequate expression reads

$$P(\varrho,\omega) \equiv F(\varrho,\omega)^2 = \mathrm{Tr}\,\varrho\,\omega + 2\sqrt{\det\varrho\,\det\omega}. \tag{43}$$

By the aid of Eq. (8) the equation can be converted to

$$C(\varrho,\omega)^2 = \mathrm{Tr}\,\varrho\,\omega - 2\sqrt{\det\varrho\,\det\omega}. \tag{44}$$

Let Θ be an antilinear Hermitian operator acting on $\mathcal{H}_2$. To get $F_\Theta(\varrho)$ or $C_\Theta(\varrho)$ we have to know the trace of $\varrho\Theta\varrho\Theta$ and the determinants of ϱ and $\Theta\varrho\Theta$.

After these preliminaries we think of $\mathcal{H}_2$ as of a subspace of a two-qubit Hilbert space $\mathcal{H}$. We cannot use the Hill-Wootters conjugation Θ_{HW} in Eqs. (43) or (44) directly because, generally, $\mathcal{H}_2$ will not allow Θ_{HW} as a symmetry. Therefore we set $\Theta := Q\Theta_{HW}Q$ with Q the projection operator projecting $\mathcal{H}$ onto $\mathcal{H}_2$. Θ, so defined, will be antilinearly Hermitian and it maps $\mathcal{H}_2$ into $\mathcal{H}_2$. By the little trick we see, abbreviating $\tilde{\varrho} = \Theta_{HW}\varrho\Theta_{HW}$,

$$F(\varrho,\tilde{\varrho}) = F_\Theta(\varrho), \quad C(\varrho,\tilde{\varrho}) = C_\Theta(\varrho)$$

whenever ϱ is supported by $\mathcal{H}_2$.

We assume $\mathcal{H}_2$ is generated by two separable unit vectors

$$\psi_i = \phi_i^a\otimes\phi_i^b \in \mathcal{H} = \mathcal{H}^a\otimes\mathcal{H}^b. \tag{45}$$

We choose their phases such that

$$\langle\phi_0^a,\phi_1^a\rangle = a, \quad \langle\phi_0^b,\phi_1^b\rangle = b, \tag{46}$$

where a, b are positive real numbers between 0 and 1. We get, by appropriately adjusting the free phase in the Hill-Wootters conjugation

$$\langle\psi_1,\Theta_{HW}\psi_0\rangle = \langle\psi_0,\Theta_{HW}\psi_1\rangle = \sqrt{(1-a^2)(1-b^2)}. \tag{47}$$

We can replace Θ_{HW} by $\Theta = Q\Theta_{HW}Q$ in Eq. (47) without changing its validity. This reminds us also that $\langle\psi_i,\Theta\psi_i\rangle = 0$ because ψ_i is a product vector.

We introduce a suitable basis by

$$\varphi^+=\frac{\psi_0+\psi_1}{\sqrt{2(1+ab)}},\quad \varphi^-=\frac{\psi_0-\psi_1}{\sqrt{2(1-ab)}}. \tag{48}$$

By a short calculation one concludes from Eq. (47)

$$\Theta\varphi^\pm=a_\pm\varphi^\pm,\quad a_\pm=\frac{\sqrt{(1-a^2)(1-b^2)}}{1\pm ab}. \tag{49}$$

Possessing a distinguished basis (48) in $\mathcal{H}_2$ we represent any density operator ϱ supported by $\mathcal{H}_2$ as usual by the help of Pauli operators, see Eq. (1). The Pauli operators to the basis (49) are by convention

$$\sigma_3=|\varphi^+\rangle\langle\varphi^+|-|\varphi^-\rangle\langle\varphi^-|,\sigma_1=|\varphi^+\rangle\langle\varphi^-|+|\varphi^-\rangle\langle\varphi^+|$$

and $\sigma_2=i\sigma_1\sigma_3$. Transforming ϱ according to $\varrho\to\Theta\varrho\Theta$ can be accomplished by transforming the identity of $\mathcal{H}_2$ and the just introduced Pauli operators. Using Eq. (49),

$$\Theta^2=\Theta Q\Theta=\frac{a_+^2+a_-^2}{2}\mathbf{1}+\frac{a_+^2-a_-^2}{2}\sigma_3,$$

$$\Theta\sigma_3\Theta=\frac{a_+^2-a_-^2}{2}\mathbf{1}+\frac{a_+^2+a_-^2}{2}\sigma_3,$$

$$\Theta\sigma_1\Theta=a_+a_-\sigma_1,\quad \Theta\sigma_2\Theta=-a_+a_-\sigma_2.$$

One gets for the determinant

$$\det\Theta\varrho\Theta=(a_+a_-)^2\det\varrho.$$

and for the trace of $\varrho\Theta\varrho\Theta$

$$\frac{a_+^2+a_-^2}{4}(x_0^2+x_3^2)+\frac{a_+^2-a_-^2}{2}x_0x_3+\frac{a_+a_-}{2}(x_1^2-x_2^2).$$

These expressions shall be inserted into Eqs. (43) and (44):

$$F_\Theta(\varrho)^2=\tfrac{1}{4}[(a_++a_-)x_0+(a_+-a_-)x_3]^2-a_+a_-x_2^2,$$

$$C_\Theta(\varrho)^2=\tfrac{1}{4}[(a_+-a_-)x_0+(a_++a_-)x_3]^2+a_+a_-x_1^2.$$

One should have in mind $x_0=1$ for normalized density operators. Then the last equation represents just Wootters concurrence $C(\varrho)$ for density operators supported by $\mathcal{H}_2$. Returning to the amplitudes (46), a and b, results in a more convenient form

$$F_\Theta(\varrho)=A\sqrt{(x_0-abx_3)^2-(1-a^2b^2)x_2^2}, \tag{50}$$

$$C_\Theta(\varrho)=A\sqrt{(x_3-abx_0)^2+(1-a^2b^2)x_1^2}, \tag{51}$$

$$A:=\sqrt{\frac{(1-a^2)(1-b^2)}{1-a^2b^2}}. \tag{52}$$

One easily determines to convex leaves for these roofs: For F_Θ we fix $x_0=1$, x_2, and x_3 and let x_1 vary. We obtain a straight line in x-space which intersects the Bloch sphere of $\mathcal{H}_2$ exactly twice, corresponding to the two x_3-values with which x_1,x_2,x_3 becomes a unit vector. Along the line the Θ fidelity remains constant. The same procedure, however, with fixing x_0,x_1,x_3 and varying x_2, produces the convex foliation for the Θ concurrence which, in our example, is the Hill, Wootters one.

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