Joint Schmidt-type decomposition for two bipartite pure quantum states

Christopher Eltschka[1] and Jens Siewert[2,3]
[1]*Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany*
[2]*Departamento de Química Física, Universidad del País Vasco UPV/EHU, E-48080 Bilbao, Spain*
[3]*IKERBASQUE Basque Foundation for Science, E-48013 Bilbao, Spain*

(Received 2 April 2019; revised manuscript received 18 December 2019; accepted 17 January 2020; published 3 February 2020)

It is well known that the Schmidt decomposition exists for all pure states of a two-party quantum system. We demonstrate that there are two ways to obtain an analogous decomposition for arbitrary rank-1 operators acting on states of a bipartite finite-dimensional Hilbert space. These methods amount to joint Schmidt-type decompositions of two pure states where the two sets of coefficients and local bases depend on the properties of either state, however, at the expense of the local bases not all being orthonormal and in one case the complex-valuedness of the coefficients. With these results we derive several generally valid purity-type formulas for one-party reductions of rank-1 operators, and we point out relevant relations between the Schmidt decomposition and the Bloch representation of bipartite pure states.

DOI: 10.1103/PhysRevA.101.022302

I. INTRODUCTION

The Schmidt decomposition theorem states that any pure state of a bipartite quantum system of finite dimension can be written as the superposition of a minimum number of states, where the coefficients are real and the superposed states are tensor products of the elements of two preferred local orthonormal bases. There are only a few tools in quantum information theory comparable in the power of the method and the ubiquity of their applicability with the Schmidt decomposition. While Schmidt's original work [1] investigates kernels of integral equations, the decomposition for finite-dimensional systems—as it is mostly applied in quantum physics nowadays—was given by Everett III [2,3].

There are several routes toward generalization of the method. There is a mixed-state analog [4,5], which is not as frequently used as the pure-state decomposition [6], but has important applications, e.g., in decomposition of quantum gates and entanglement theory [7,8]. Further, it would be desirable to have a similar method for multipartite states, e.g., [9–12]. While for three qubits this question has lead to important results [13], to date there is no generally accepted counterpart for the Schmidt decomposition in multipartite systems.

A third option is to ask whether there exists a simultaneous Schmidt-type decomposition for several pure bipartite states. In Ref. [14], the conditions for simultaneous applicability of a (slightly generalized) standard Schmidt decomposition were studied; mixtures of such jointly Schmidt-decomposable states (that is, Schmidt-decomposable in one and the same pair of local bases) were then called maximally correlated. However, beyond this restrictive concept nothing seems to be known regarding simultaneous Schmidt decomposability of two or more bipartite states. The reason for this is that in general the reduced states have nonvanishing overlap and therefore it is not obvious which basis one has to choose in the subspace of their joint support. Our present work fills this gap by analyzing the question of how two pairs of correlated local bases can be found that allow for Schmidt-like decompositions of two arbitrary finite-dimensional bipartite states. We show that in general there are two options for such decomposability and that those generalized Schmidt bases differ from the standard—"single-state"—Schmidt bases whenever the reduced states have nonvanishing overlap. As a direct consequence of these results we derive several interesting relations for the reductions of rank-1 operators. As the Schmidt decomposition, the existence of relations for one-party reductions, and the Bloch representation [15–22] of bipartite quantum states are intimately related concepts [19,21,23], we conclude our discussion by analyzing the most salient of these mathematical connections.

II. THE USUAL SCHMIDT DECOMPOSITION

We start with a brief reminder of how the Schmidt decomposition is obtained following Preskill [24]. Consider the generic normalized state $|\psi_{AB}\rangle$ of a bipartite Hilbert space, $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, $\langle\psi_{AB}|\psi_{AB}\rangle = 1$. We write it with respect to some orthonormal product bases as

$$|\psi_{AB}\rangle = \sum_{j,k=1}^{d} a_{jk}|j\rangle_A \otimes |k\rangle_B \equiv \sum_j |j\rangle_A \otimes |\tilde{j}\rangle_B, \qquad (1)$$

where the states $|\tilde{j}\rangle_B$ in general are neither normalized nor orthogonal. If we choose, however, for $\{|j\rangle_A\}$ the basis in which the reduced state

$$\rho_A = \mathrm{Tr}_B\,|\psi_{AB}\rangle\langle\psi_{AB}| = \sum_{jk}\langle\tilde{k}|\tilde{j}\rangle\,|j\rangle_A\langle k|$$

is diagonal, the states $\{|\tilde{j}\rangle_B\}$ do become orthogonal, and by introducing $|j'\rangle_B = \lambda_j^{-1/2}|\tilde{j}\rangle_B$ for $\lambda_j = \langle\tilde{j}|\tilde{j}\rangle > 0$, we get the

Schmidt decomposition of $|\psi_{AB}\rangle$:

$$|\psi_{AB}\rangle = \sum_{j,k=1}^{d} \sqrt{\lambda_j}|j\rangle_A \otimes |j'\rangle_B, \quad \sum_j \lambda_j = 1. \tag{2}$$

It is an immediate consequence that with this choice of local bases also $\rho_B = \mathrm{Tr}_A\, |\psi_{AB}\rangle\langle\psi_{AB}|$ is diagonal and has the same set of nonzero eigenvalues $\{\lambda_j\}$ as ρ_A, so that one finds for the purities of the local states the well-known relation

$$\mathrm{Tr}\, \rho_A^2 = \mathrm{Tr}\, \rho_B^2 = \sum_j \lambda_j^2. \tag{3}$$

III. DECOMPOSITION OF RANK-1 OPERATORS

A. Decomposition based on singular value decomposition

The Schmidt decomposition, Eq. (2), for a projector $|\psi_{AB}\rangle\langle\psi_{AB}|$ reads

$$|\psi_{AB}\rangle\langle\psi_{AB}| = \sum_{jk} \sqrt{\lambda_j\lambda_k}|a_j\rangle_A\langle a_k| \otimes |b_j\rangle_B\langle b_k|, \tag{4}$$

with the Schmidt basis $\{|a_j\rangle_A \otimes |b_k\rangle_B\}$. This way of writing the decomposition imposes the following question: What happens if, in the expression $|\psi_{AB}\rangle\langle\psi_{AB}|$, we do not choose both sides equal; that is, is there an analogous expansion for the—non-Hermitian—rank-1 operator $|\psi_{AB}\rangle\langle\phi_{AB}|$ with $|\phi_{AB}\rangle \neq |\psi_{AB}\rangle$? An obvious idea would be to resort to the operator-level Schmidt decompositon; however, this way one simply retrieves the usual Schmidt decompsition of the individual states (cf. Ref. [6]).

In order to find a new answer we assume that $|\psi_{AB}\rangle, |\phi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ are normalized and make an ansatz similar to what we had in Eq. (1):

$$|\psi_{AB}\rangle = \sum_j |u_j\rangle_A|\tilde{j}^{\psi}\rangle_B, \tag{5a}$$

$$|\phi_{AB}\rangle = \sum_k |v_k\rangle_A|\tilde{k}^{\phi}\rangle_B, \tag{5b}$$

where $\{|u_j\rangle_A\}$ and $\{|v_k\rangle_A\}$ are orthonormal bases (from now on we drop the tensor product signs and the lower indices for the partitions A and B). If we choose the bases $\{|u_j\rangle\}$ and $\{|v_k\rangle\}$ such that they belong to the singular value decomposition (SVD) of $\mathrm{Tr}_B\, |\psi\rangle\langle\phi|$ with singular values $q_j \geqq 0$, the marginal operator for party A reads

$$\mathrm{Tr}_B\, |\psi\rangle\langle\phi| = \sum_{jk} |u_j\rangle\langle v_k|\langle\tilde{k}^{\phi}|\tilde{j}^{\psi}\rangle = \sum_j q_j|u_j\rangle\langle v_j|, \tag{6}$$

with $\langle\tilde{k}^{\phi}|\tilde{j}^{\psi}\rangle = q_j\delta_{jk}$. That is, we find that $\{|\tilde{j}^{\psi}\rangle\}$ and $\{|\tilde{k}^{\phi}\rangle\}$ are dual bases. If we normalize as before

$$\left|\mathsf{d}_j^{\psi}\right\rangle \equiv \frac{|\tilde{j}^{\psi}\rangle}{\sqrt{\mu_j^{\psi}}}, \quad \left|\mathsf{d}_k^{\phi}\right\rangle \equiv \frac{|\tilde{k}^{\phi}\rangle}{\sqrt{\nu_k^{\phi}}},$$

we can finally write the following for the decomposition of $|\psi\rangle$ and $|\phi\rangle$:

$$|\psi\rangle = \sum_j \sqrt{\mu_j^{\psi}}|u_j\rangle\left|\mathsf{d}_j^{\psi}\right\rangle, \tag{7a}$$

$$|\phi\rangle = \sum_k \sqrt{\nu_k^{\phi}}|v_k\rangle\left|\mathsf{d}_k^{\phi}\right\rangle. \tag{7b}$$

One can term this the SVD-based simultaneous Schmidt-like decomposition of $|\psi\rangle$ and $|\phi\rangle$. We recognize the analogy of Eqs. 7(a) and 7(b) with the usual Schmidt decomposition Eq. (2). Note that, while the generalized "Schmidt coefficients" μ_j^{ψ} and ν_k^{ϕ} are still real, only the bases $\{|u_j\rangle\}$ and $\{|v_k\rangle\}$ are orthonormal. The normalized bases $\{|\mathsf{d}_j^{\psi}\rangle\}$ and $\{|\mathsf{d}_k^{\phi}\rangle\}$ are dual with $\sqrt{\mu_j^{\psi}\nu_k^{\phi}}\langle\mathsf{d}_j^{\psi}|\mathsf{d}_k^{\phi}\rangle = q_j\delta_{jk}$, but not orthogonal. It is worthwhile noting that in general the orthonormal bases $\{|u_j\rangle\}$ and $\{|v_k\rangle\}$ bear no special relation with one another. Again, Eqs. (7) represent superpositions with the minimum number of components, which equals the rank of the reduced operator $\mathrm{Tr}_B\, |\psi\rangle\langle\phi|$. As the "Schmidt vectors" in Eqs. (7) are still orthogonal we have $\sum_j \mu_j^{\psi} = \sum_k \nu_k^{\phi} = 1$. Moreover, there is the condition $\sum_j q_j\langle v_j|u_j\rangle = \langle\phi|\psi\rangle$. Clearly, one finds an analogous decomposition with exchanged roles of parties A and B by considering the reduced operator $\mathrm{Tr}_A\, |\psi\rangle\langle\phi|$ and modifying Eqs. (5) correspondingly.

The decompositions, Eqs. (7), may be viewed as the result of selecting preferred local bases for $|\psi\rangle$ and $|\phi\rangle$ depending on the overlap of these bipartite states on party B only. This dependence does not exist if $\mathrm{Tr}_B\, |\psi\rangle\langle\phi| = 0$. We discuss this case below.

B. Decomposition based on diagonalization

Interestingly, Eqs. (7) are not the only way to obtain a joint Schmidt-like decomposition of two pure states. To see this, we start with an ansatz similar to Eqs. (5) where we drop the assumption that the bases on party A be orthonormal:

$$|\psi\rangle = \sum_j |x_j\rangle|\tilde{j}^{\psi}\rangle, \tag{8a}$$

$$|\phi\rangle = \sum_k |y_k\rangle|\tilde{k}^{\phi}\rangle. \tag{8b}$$

The trick that led to the decomposition was to find a diagonal form of the reduced operator $\mathrm{Tr}_B\, |\psi\rangle\langle\phi|$, which was achieved via the singular value decomposition. There is an alternative to this approach, namely to diagonalize $\mathrm{Tr}_B\, |\psi\rangle\langle\phi|$. Note that diagonalizability of non-Hermitian matrices is not guaranteed. A sufficient condition is that $\mathrm{Tr}_B\, |\psi\rangle\langle\phi|$ has the maximum number of nonzero eigenvalues, which all have to be different [25].

Hence we assume that a matrix representation M of $\mathrm{Tr}_B\, |\psi\rangle\langle\phi|$ is similar to a diagonal matrix D

$$\mathsf{M} = \mathsf{S}\cdot\mathsf{D}\cdot\mathsf{S}^{-1},$$

where S is an invertible matrix. The columns of S are the right eigenvectors of M, whereas the rows of S^{-1} are the left eigenvectors. Correspondingly we can write the reduced operator

$$\mathrm{Tr}_B\, |\psi\rangle\langle\phi| = \sum_j \Delta_j e^{i\varphi_j}|\mathsf{s}_j\rangle\langle\mathsf{s}_j^{-1}|, \tag{9}$$

where $\{|\mathsf{s}_j\rangle\}$ and $|\mathsf{s}_k^{-1}\rangle\}$ are (nonorthogonal) dual bases of $\mathcal{H}_A$, i.e., $\langle\mathsf{s}_j|\mathsf{s}_k^{-1}\rangle = \delta_{jk}$. Note that $(\langle\mathsf{s}_j^{-1}|)^{\dagger} \neq |\mathsf{s}_j\rangle$. Moreover, we have explicitly written the phases of the eigenvalues implying that $\Delta_j \geqq 0$.

In analogy with the discussion following Eq. (6), we then find that $|\tilde{j}^{\psi}\rangle$ and $|\tilde{k}^{\phi}\rangle$ are proportional to the vectors of the two dual bases $\{|\mathsf{t}_j\rangle\}$ and $\{|\mathsf{t}_k^{-1}\rangle\}$, with $\langle \mathsf{t}_j|\mathsf{t}_k^{-1}\rangle = \delta_{jk}$, so that we arrive at

$$|\psi\rangle = \sum_j \sqrt{\xi_j}|\mathsf{s}_j\rangle|\mathsf{t}_j\rangle, \tag{10a}$$

$$|\phi\rangle = \sum_k \sqrt{\eta_k}e^{-i\varphi_k}\big|\mathsf{s}_k^{-1}\big\rangle\big|\mathsf{t}_k^{-1}\big\rangle, \tag{10b}$$

with $\xi_j, \eta_k \geqq 0$ and $\sqrt{\xi_j\eta_j} = \Delta_j$. Equations (10) represent the second simultaneous Schmidt-like decomposition of $|\psi\rangle$ and $|\phi\rangle$, which now is diagonalization based. Here, the "Schmidt coefficients" have complex phases, but there is a freedom to distribute each of the phases at will among the two states. Interestingly, both reduced operators $\mathrm{Tr}_A\,|\psi\rangle\langle\phi|$ and $\mathrm{Tr}_B\,|\psi\rangle\langle\phi|$ have the same nonzero (now complex) eigenvalues $\{\Delta_j e^{i\varphi}\}$, analogously to the usual Schmidt decomposition of a single state. Since the "Schmidt vectors" are not orthogonal, there is no normalization condition for ξ_j and η_k. In contrast to the decomposition in Eqs. (7), both of the local bases of $|\psi\rangle$ are strongly related with the corresponding basis in $|\phi\rangle$; however, none of them are necessarily orthogonal or normalized. We stress again that the decomposition in Eqs. (10) may not exist, while the decomposition in Eqs. (7) can always be found; hence the latter is the stronger statement.

C. Remarks and special cases

The obvious special case for the decompositions in Eqs. (7) and (10) is equality, $|\psi\rangle = |\phi\rangle$. Here we get back the known result, Eq. (2), because the dual bases become self-dual and therefore also orthonormal. For Hermitian matrices the singular value decomposition coincides with diagonalization; this ensures the usual Schmidt decomposition also for the first generalization option.

One might expect that also the orthogonality $\langle\phi|\psi\rangle = 0$ represents a special case, but as long as the reduced operators $\mathrm{Tr}_A\,|\psi\rangle\langle\phi|$ and $\mathrm{Tr}_B\,|\psi\rangle\langle\phi|$ do not vanish, the resulting bases do not display special properties.

However, there is a case related to orthogonality $\langle\phi|\psi\rangle = 0$ that needs to be discussed: the possibility that $\mathrm{Tr}_A\,|\psi\rangle\langle\phi| = 0$ or/and $\mathrm{Tr}_B\,|\psi\rangle\langle\phi| = 0$. Any of these conditions imply global orthogonality, because, e.g., $\langle\phi|\psi\rangle = \mathrm{Tr}\,(\,\mathrm{Tr}_B\,|\psi\rangle\langle\phi|) = 0$. With the latter condition, for example, our approach to derive Eqs. (7) or Eqs. (10), respectively, does not lead to the selection of preferred bases on party A. For $\mathrm{Tr}_B\,|\psi\rangle\langle\phi| = 0$, the states $|\psi\rangle$ and $|\phi\rangle$ have disjoint support in $\mathcal{H}_B$, implying also that none of them has full (usual) Schmidt rank. Another consequence is orthogonality of the local states, $\mathrm{Tr}\,[\,\mathrm{Tr}_A\,|\psi\rangle\langle\psi|\,\mathrm{Tr}_A\,|\phi\rangle\langle\phi|] = 0$.

In the case of disjoint support on $\mathcal{H}_B$ one can try to check $\mathrm{Tr}_A\,|\psi\rangle\langle\phi|$; if it is nonzero the simultaneous Schmidt decomposition can be found as shown before, that is, with dual bases in $\mathcal{H}_A$ and singular value decomposition (or diagonalization) in $\mathcal{H}_B$. If, however, also $\mathrm{Tr}_A\,|\psi\rangle\langle\phi| = \mathrm{Tr}_B\,|\psi\rangle\langle\phi| = 0$, the states have disjoint support on the entire composite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, and it is not possible (but also not necessary) to select preferred local bases whose properties depend on both $|\psi\rangle$ and $|\phi\rangle$. It suffices then to diagonalize the local states of $|\psi\rangle$ and $|\phi\rangle$ separately and to use their standard Schmidt decomposition.

IV. GENERALIZED PURITY RELATIONS

As an immediate application of the decomposition equations, Eqs. (7) and (10), we derive several formulas that may be regarded as the generalizations of the purity relation, Eq. (3).

Consider first the squares of the reduced rank-1 operators. By using Eq. (6) we find $\mathrm{Tr}\,(\,\mathrm{Tr}_B\,|\psi\rangle\langle\phi|)^2 = \sum_{jk} q_j q_k \langle v_j|u_k\rangle\langle v_k|u_j\rangle$. On the other hand, $\mathrm{Tr}_A\,|\psi\rangle\langle\phi| = \sum_{jk}(\mu_j^{\psi}\nu_k^{\phi})^{1/2}\langle v_k|u_j\rangle|\mathsf{d}_j^{\psi}\rangle\langle\mathsf{d}_k^{\phi}|$. Because of $(\mu_j^{\psi}\nu_k^{\phi})^{1/2}\langle\mathsf{d}_k^{\phi}|\mathsf{d}_j^{\psi}\rangle = q_j\delta_{jk}$, it follows that

$$\begin{aligned}\mathrm{Tr}(\mathrm{Tr}_A\,|\psi\rangle\langle\phi|)^2 &= \sum_{jklm}\sqrt{\mu_j^{\psi}\nu_k^{\phi}}\sqrt{\mu_l^{\psi}\nu_m^{\phi}} \\ &\quad\times\langle v_k|u_j\rangle\langle v_m|u_l\rangle\big\langle\mathsf{d}_k^{\phi}|\mathsf{d}_l^{\psi}\big\rangle\big\langle\mathsf{d}_m^{\phi}|\mathsf{d}_j^{\psi}\big\rangle \\ &= \sum_{jk} q_j q_k\langle v_j|u_k\rangle\langle v_k|u_j\rangle,\end{aligned}$$

so that we conclude

$$\mathrm{Tr}(\mathrm{Tr}_A\,|\psi\rangle\langle\phi|)^2 = \mathrm{Tr}(\mathrm{Tr}_B\,|\psi\rangle\langle\phi|)^2. \tag{11}$$

If the reduced operators are diagonalizable, Eq. (11) follows practically without calculation, because $\mathrm{Tr}_A\,|\psi\rangle\langle\phi|$ and $\mathrm{Tr}_B\,|\psi\rangle\langle\phi|$ have the same (in general, complex) eigenvalues.

Alternatively, one can read Eq. (3) as Hilbert-Schmidt scalar products. Then, we derive in a completely analogous manner the second generalized purity relation:

$$\begin{aligned}\mathrm{Tr}[\mathrm{Tr}_B\,|\psi\rangle\langle\phi|\,\mathrm{Tr}_B\,|\phi\rangle\langle\psi|] &= \sum_j q_j^2 \\ &= \mathrm{Tr}[\mathrm{Tr}_A\,|\psi\rangle\langle\psi|\,\mathrm{Tr}_A\,|\phi\rangle\langle\phi|].\end{aligned} \tag{12}$$

We can go one step further and turn Eqs. (11) and (12) into a single equality linking the reductions of four bipartite states $\psi, \phi, \chi, \zeta \in \mathcal{H}_A \otimes \mathcal{H}_B$:

$$\mathrm{Tr}[\mathrm{Tr}_A\,|\psi\rangle\langle\chi|\,\mathrm{Tr}_A\,|\phi\rangle\langle\zeta|] = \mathrm{Tr}[\mathrm{Tr}_B\,|\psi\rangle\langle\zeta|\,\mathrm{Tr}_B\,|\phi\rangle\langle\chi|]. \tag{13}$$

The relations Eqs. (11)–(13) constitute the second central result of our article. They are directly connected with the Bloch representation of quantum states; therefore they are highly useful in calculations within that formalism, as will be demonstrated in forthcoming work. We highlight some of the links to the Bloch representation in the last part of our discussion.

V. SCHMIDT DECOMPOSITION AND BLOCH REPRESENTATION

Our main point in generalizing the Schmidt decomposition was to consider rank-1 operators such as $|\psi\rangle\langle\phi|$ and $|\psi\rangle\langle\psi|$ rather than state vectors like $|\psi\rangle$. Moreover, we have seen in the preceding sections that a discussion of the Schmidt decomposition (both the usual version and the joint version) is closely related to analyzing the properties of the marginals. Thus one is led to associate the entire discussion with yet another topic where operators and their marginals are intrinsically tied together, namely the Bloch representation of quantum states. This link is rarely emphasized; therefore we use this section to work out some of its details. We restrict this analysis mainly to properties of the usual (single-state) Schmidt decompostion (cf. Sec. II): however, some of the results we derived earlier turn out to be useful. In our considerations we assume Hilbert spaces of equal dimension, $\dim\mathcal{H}_A = \dim\mathcal{H}_B = d$ (this can always be achieved by extending the Hilbert space of lower dimension), because it makes the expressions more transparent.

The Bloch representation of bipartite states is defined as follows (cf., e.g., Refs. [15–22]): Given an orthonormal basis of trace-free Hermitian matrices $\{\mathsf{h}_j\}$ [with normalization $\mathrm{Tr}\,(\mathsf{h}_j\mathsf{h}_k) = d\,\delta_{jk}$ and $\mathsf{h}_0 \equiv \mathbb{1}$] we can expand any density operator ρ acting on $\mathcal{H}_A\otimes\mathcal{H}_B$

$$\rho = \frac{1}{d^2}\Bigg[(\mathrm{Tr}\,\rho)\mathbb{1}\otimes\mathbb{1} + \sum_{j=1}^{d^2-1} r_{j0}\mathsf{h}_j\otimes\mathbb{1} + \sum_{k=1}^{d^2-1} r_{0k}\mathbb{1}\otimes\mathsf{h}_k + \sum_{l,m=1}^{d^2-1} r_{lm}\mathsf{h}_l\otimes\mathsf{h}_m\Bigg]. \tag{14}$$

With the simplifying choice of Hermitian matrices h_j the coefficients r_{j0}, r_{0k}, and r_{lm} are real. We call the sum of terms with one summation index "1-sector," and the one with two indices "2-sector." The first term on the right-hand side of Eq. (14) can be denoted the "0-sector," accordingly. The purity condition for the state ρ translates into the Bloch vector length as the sum of sector lengths [19–22]:

$$d^2\,\mathrm{Tr}\,\rho^2 = (\mathrm{Tr}\,\rho)^2 + \sum_{j=1}^{d^2-1} r_{j0}^2 + \sum_{k=1}^{d^2-1} r_{0k}^2 + \sum_{l,m=1}^{d^2-1} r_{lm}^2. \tag{15}$$

Each of the sums in Eq. (15) is invariant under local unitary transformations [26]. The purity condition (3) for the reduced states corresponds to the equality of the normalized 1-sector lengths $\sum_j r_{j0}^2 = \sum_k r_{0k}^2$. Moreover, we note that for normalized states $\sum_{j,k=0}^{d^2-1} r_{jk}^2 \leqq d^2$.

Consider now the Bloch representation of the rank-1 operator $|\psi\rangle\langle\phi|$,

$$|\psi\rangle\langle\phi| = \frac{1}{d^2}\sum_{lm} x_{lm}\mathsf{h}_l\otimes\mathsf{h}_m.$$

The coefficients x_{jk} in general are complex. For normalized $|\psi\rangle$ and $|\phi\rangle$, it follows that $\mathrm{Tr}\,[(|\psi\rangle\langle\phi|)^\dagger|\psi\rangle\langle\phi|] = 1$; hence the total length of this rank-1 operator is

$$\sum_{j,k=0}^{d^2-1} |x_{jk}|^2 = d^2. \tag{16}$$

With our discussion above and Eq. (12) we find that in general $\sum_j |x_{j0}|^2 \neq \sum_k |x_{0k}|^2$. For example, it is well possible that $\sum_{j=0}^{d^2-1} |x_{j0}|^2 = 0$ while still $\sum_{k=0}^{d^2-1} |x_{0k}|^2 \neq 0$. As we discussed, $\mathrm{Tr}_B\,|\psi\rangle\langle\phi| = 0$ implies $\langle\psi|\phi\rangle = 0$; hence in this case the Bloch representation consists only of the 1-sector corresponding to party B and the 2-sector. If both $\mathrm{Tr}_A\,|\psi\rangle\langle\phi| = \mathrm{Tr}_B\,|\psi\rangle\langle\phi| = 0$, only the 2-sector has nonvanishing components.

The Schmidt decomposition in a way captures the essence of superposition for bipartite states. On the other hand, for density operators—as described by the Bloch representation—superposition is not a concept as obvious as for state vectors. Let us therefore elaborate further on the properties of superpositions in the Bloch formalism. Consider the superposition of several normalized orthogonal states $|\phi_j\rangle \in \mathcal{H}_A\otimes\mathcal{H}_B$, $1 \leqq j \leqq d^2$

$$|\Psi\rangle = \sum_j a_j|\phi_j\rangle. \tag{17}$$

The projector onto $|\Psi\rangle$ naturally splits up into a diagonal and an off-diagonal part, $|\Psi\rangle\langle\Psi| = \mathsf{diag} + \mathsf{offdiag}$,

$$\mathsf{diag} = \sum_j |a_j|^2|\phi_j\rangle\langle\phi_j|, \tag{18a}$$

$$\mathsf{offdiag} = \sum_{j<k} a_j a_k^*|\phi_j\rangle\langle\phi_k| + a_j^* a_k|\phi_k\rangle\langle\phi_j|, \tag{18b}$$

which are orthogonal $\mathrm{Tr}\,(\mathsf{diag}^\dagger\mathsf{offdiag}) = 0$. Hence, for the Bloch vector length of $|\Psi\rangle\langle\Psi|$ divided by d^2 we have $1 = \mathrm{Tr}\,(\mathsf{diag}^\dagger\mathsf{diag}) + \mathrm{Tr}\,(\mathsf{offdiag}^\dagger\mathsf{offdiag}) = \sum_j |a_j|^4 + 2\sum_{j<k}|a_j|^2|a_k|^2$.

For bipartite systems one commonly chooses $|\phi_j\rangle$ in Eq. (17) as tensor products of local basis states in order to distinguish local from nonlocal physics. It is then convenient to use two summation indices $|\Psi\rangle = \sum_{kl} a_{kl}|e_k f_l\rangle$ with local orthonormal bases $\{|e_k\rangle\}$ and $\{|f_l\rangle\}$ $(k, l = 1,\dots,d)$. The matrices $\{\mathsf{h}_j\}$ (e.g., the generalized Gell-Mann matrices [22]) refer to the same local bases. Among all the possible local bases the (usual) Schmidt basis of $|\Psi\rangle$ is peculiar: $|e_k f_k\rangle$ become the Schmidt vectors and $a_{kl} \longrightarrow \sqrt{\lambda_k}\,\delta_{kl}$ the Schmidt coefficients. As then $\mathrm{Tr}_A\,|\Psi\rangle\langle\Psi|$ and $\mathrm{Tr}_B\,|\Psi\rangle\langle\Psi|$ are diagonal, the Bloch representation of $|\Psi\rangle\langle\Psi|$ contains only diagonal matrix terms in the 1-sector. Remarkably, the length $\mathrm{Tr}\,(\mathsf{offdiag}^\dagger\mathsf{offdiag}) = 2\sum_{j<k}\lambda_j\lambda_k$ equals half the squared concurrence of $|\Psi\rangle$ [27].

In Eq. (18) we can recognize the importance of the second generalized purity relation, Eq. (12): If one wants to describe the parts of a superposition in terms of the Bloch vector coefficients of the superposed states $|\phi_j\rangle\langle\phi_j|$, this is obvious for the diagonal part. In contrast, it is not clear whether there is any simple relation between the rank-1 operators in $\mathsf{offidag}$ [cf. Eq. (18a)] and the Bloch coefficients. Here, Eq. (12) provides an answer.

We may ask what the contributions of diag and $\mathsf{offdiag}$ to the sectors of the Bloch representation are. Both 1- and 2-sector lengths are invariant under local unitaries; therefore a local basis change leads to a redistribution of the parts that diag and $\mathsf{offdiag}$ contribute to the 1-sector or the 2-sector, respectively. The Schmidt decomposition is special, because $\mathrm{Tr}_A\,(|e_k f_k\rangle\langle e_l f_l|) = \mathrm{Tr}_B\,(|e_k f_k\rangle\langle e_l f_l|) = 0$ (for $k \neq l$); that is, $\mathsf{offdiag}$ does not contribute to the 1-sector at all, while (trivially) the diag contribution to the 1-sector is maximum. However, a nontrivial fact is that the diag contribution to the 2-sector also has its maximum in the Schmidt basis (for the

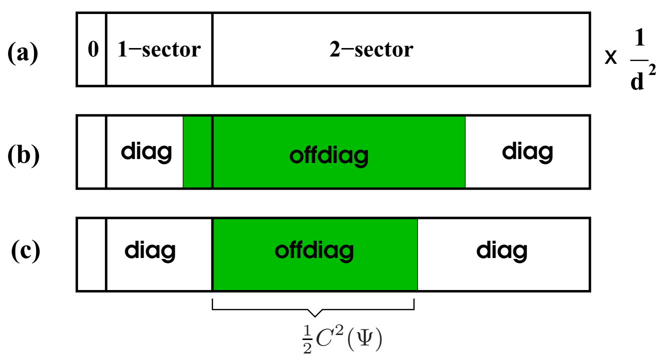

FIG. 1. Schematic of the diag/offdiag contributions to the 1-sector/2-sector of $|\Psi\rangle\langle\Psi|$ for different choices of local bases. The 0-sector per definition belongs to diag. (a) The lengths of the 0-sector, the 1-sector, and the 2-sector are invariant under local basis changes. (b) Generic local bases: diag and offdiag contribute to both the 1-sector and the 2-sector. (c) Schmidt basis: offdiag does not contribute to the 1-sector and has minimum length, which equals half the squared concurrence $\frac{1}{2}C^2(\Psi)$. The diag contribution to the 2-sector is maximum. Correspondingly, also the total length of diag is maximum. The total length of all contributions in this figure is 1 [note that the sum of sector lengths, Eq. (15), per definition equals d^2].

proof, see Appendix),

$$\mathrm{Tr}[(\text{2-sector})\mathsf{diag}] \underset{\text{Schmidt decomp.}}{\longrightarrow} \max, \tag{19a}$$

$$\mathrm{Tr}[(\text{2-sector})\mathsf{offdiag}] \underset{\text{Schmidt decomp.}}{\longrightarrow} \min, \tag{19b}$$

where “2-sector” $= \sum_{jk} r_{jk}\mathsf{h}_j \otimes \mathsf{h}_k$, as defined as before in Eq. (14), so that the entire diag length is maximum in the Schmidt basis, whereas the offdiag length is minimum and equals half of the squared concurrence (cf. Fig. 1).

This illustrates an archetypical situation for the Bloch formalism: In a parametrically interesting regime (here, the special choice of the Schmidt bases), various relevant quantities assume extreme values, such as the total diag length and the 1-sector diag contribution. However, intriguingly, also the difference of these maximum values, the 2-sector diag part, is *maximum*. We mention that this fact was observed independently by Huber [28].

VI. CONCLUSIONS

We have devised two ways to obtain a simultaneous Schmidt-type decomposition of two arbitrary bipartite pure states in finite dimensions, Eqs. (7) and (10), based on singular value decomposition of the reduced rank-1 operator, on the one hand, and on diagonalization thereof, on the other. The corresponding “Schmidt bases” depend on the overlap of the reduced states in the local Hilbert spaces; consequently, if there is no overlap one can simply use the standard Schmidt decomposition. It is surprising that the simultaneous Schmidt decompositions maintain the simplicity and many of the important properties of the single-state Schmidt decomposition, such as a minimum number of (real) coefficients that equals the rank of the reduced operator. As an immediate consequence, from these decompositions we have derived several interesting purity-type relations for the reductions of bipartite pure states, Eqs. (11)–(13). Moreover we have used these results to analyze the mathematical relations between the Bloch representation and the Schmidt decomposition. To this end, we introduced the diagonal and offdiagonal operator parts diag and offdiag of a projector which make explicit the extreme properties of the Schmidt bases regarding their contribution to the sector lengths of the Bloch vector.

ACKNOWLEDGMENTS

This work was funded by the German Research Foundation under Project No. EL710/2-1, the Basque Government under Grant No. IT986-16, and MCIU/FEDER/UE under Grant No. PGC2018-101355-B-I00 (J.S.). The authors acknowledge illuminating discussions with Marcus Huber, and they acknowledge Klaus Richter's support of this project.

APPENDIX

Here we prove Eq. (19) in the main text, i.e., the statement that the contribution of diag to the 2-sector of the Bloch representation of a pure bipartite state $|\Psi\rangle = \sum_{jk} a_{jk}|jk\rangle$, $1 \leqq j, k \leqq d$, assumes its maximum for the Schmidt basis and, correspondingly, the offdiag has its minimum contribution to the 2-sector, where $\{|j\rangle\}$ and $\{|k\rangle\}$ are orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and $\sum_{jk}|a_{jk}|^2 = 1$. What we show, in fact, is the second statement, Eq. (19b). The maximum of the diag contribution to the 2-sector follows immediately by recalling that the total length of the 2-sector is invariant under local unitaries. Note that it would not be sufficient for the proof of Eq. (19) to show that the full offdiag part is minimum for the Schmidt basis.

Consider the reduced state of party A,

$$\rho_A = \mathrm{Tr}_B\,|\Psi\rangle\langle\Psi| = \sum_{jk}\left(\sum_l a_{jl}a^*_{kl}\right)|j\rangle\langle k|, \tag{A1}$$

with the diagonal elements

$$h_j = \sum_l |a_{jl}|^2. \tag{A2}$$

Assume that the Schmidt basis of $|\Psi\rangle$ on party A is

$$|e_m\rangle = \sum_n U_{mn}|n\rangle, \tag{A3}$$

where U_{mn} is a unitary matrix. In this basis ρ_A is diagonal,

$$\rho_A = \sum_j \lambda_j |e_j\rangle\langle e_j|, \tag{A4}$$

with the Schmidt coefficients λ_j of $|\Psi\rangle$. One readily obtains

$$h_j = \sum_k |U_{jk}|^2\lambda_k \equiv \sum_k M_{jk}\lambda_k, \tag{A5}$$

where the matrix M is doubly stochastic because of $|U_{jk}|^2 \geqq 0$ and $\sum_k M_{jk} = \sum_j M_{jk} = 1$. According to the Hardy-Littlewood-Pólya theorem [29] this means that the vector of Schmidt coefficients, λ, majorizes the vector $h = M\lambda$ of diagonal entries of ρ_A written in the basis $\{|j\rangle\}$,

$$\lambda \succ h. \tag{A6}$$

For a Schur concave function $f(h_1, h_2, \dots, h_d)$, Eq. (A6) implies

$$f(\lambda_1, \lambda_2, \dots, \lambda_d) \leqq f(h_1, h_2, \dots, h_d). \tag{A7}$$

Now it is known that the elementary symmetric functions are Schur concave [29]. Here we are interested in the second elementary symmetric function

$$S_2(h_1, h_2, \dots, h_d) = \sum_{j<k} h_j h_k = S_2(h). \tag{A8}$$

If we substitute Eq. (A2) and apply Eq. (A7) we obtain

$$\begin{aligned} 2\sum_{j<l} h_j h_l &= \sum_{j\neq l}\sum_{km} |a_{jk}|^2|a_{lm}|^2 \\ &\geqq \sum_{j\neq l} \lambda_j\lambda_l \qquad\qquad \text{(A9)} \\ &= \frac{1}{2}C^2(\Psi). \end{aligned}$$

Note that the summation in the first line of this equation has to be understood as

$$\sum_{k,l,m=1}^{d} \sum_{\substack{j=1 \\ j\neq l}}^{d},$$

that is, the three indices k, l, and m are summed without restriction, while the fourth index j must be different from l.

Finally we symmetrize Eq. (A9) with respect to the parties A and B (the entire discussion up to this point considered party A, but since the vector of eigenvalues is the same for ρ_B, it is equally valid for party B):

$$\begin{aligned} 2\sum_{j<l} h_j h_l &= \frac{1}{2}\left(\sum_{j\neq l, km} |a_{jk}|^2|a_{lm}|^2 + \sum_{k\neq m, jl} |a_{jk}|^2|a_{lm}|^2 \right) \\ &\geqq \sum_{j\neq l} \lambda_j\lambda_l \qquad\qquad \text{(A10)} \\ &= \frac{1}{2}C^2(\Psi). \qquad\qquad \text{(A11)} \end{aligned}$$

In order to finish the proof of Eq. (19b) we need to explain the relation of the expression in the first line of Eq. (A10) with the offdiag part in the 2-sector of $|\Psi\rangle\langle\Psi|$. The complete offdiag part is given by

$$\mathsf{offdiag}(\Psi) = \sum_{(jk)\neq(lm)} a_{jk}a_{lm}^*|jk\rangle\langle lm|, \tag{A12}$$

and, hence, its length

$$\mathrm{Tr}\left[\mathsf{offdiag}(\Psi)^\dagger \mathsf{offdiag}(\Psi)\right] = \sum_{(jk)\neq(lm)} |a_{jk}|^2|a_{lm}|^2. \tag{A13}$$

In this sum, the index pair (jk) must not coincide with the pair (lm). This is achieved by

$$\sum_{k,l,m=1}^{d} \sum_{\substack{j=1 \\ j\neq l \text{ if } k=m}}^{d} = \sum_{k,l,m=1}^{d} \sum_{\substack{j=1 \\ j\neq l}}^{d} + \sum_{j,k,l=1}^{d} \sum_{\substack{m=1 \\ m\neq k}}^{d} \delta_{jl}. \tag{A14}$$

In order to obtain the length $\ell^2_{\text{off,2-sec}}$ of the offdiag contribution to the 2-sector we need to subtract the offdiag parts of the 1-sector:

$$\begin{aligned} \ell^2_{\text{off,2-sec}} = &\sum_{(jk)\neq(lm)} |a_{jk}|^2|a_{lm}|^2 - \frac{1}{d}\sum_{j\neq l,k} |a_{jk}|^2|a_{lk}|^2 \\ &- \frac{1}{d}\sum_{j,k\neq l} |a_{jk}|^2|a_{jl}|^2. \end{aligned} \tag{A15}$$

By symmetrizing the summation rule (A14) with respect to parties A and B and applying it to Eq. (A15), we find

$$\begin{aligned} \ell^2_{\text{off,2-sec}} = &\frac{1}{2}\left(\sum_{j\neq l, km} |a_{jk}|^2|a_{lm}|^2 + \sum_{k\neq m, jl} |a_{jk}|^2|a_{lm}|^2 \right) \\ &+ \left(\frac{1}{2} - \frac{1}{d}\right)\sum_{j\neq l,k} |a_{jk}|^2|a_{lk}|^2 \\ &+ \left(\frac{1}{2} - \frac{1}{d}\right)\sum_{j,k\neq l} |a_{jk}|^2|a_{jl}|^2. \end{aligned} \tag{A16}$$

Thus, since $d \geqq 2$, the sum in Eq. (A16) contains more (nonnegative) terms than the one in Eq. (A10), so that

$$\ell_{\text{off,2-sec}} \geqq 2\sum_{j<l} h_j h_l \geqq 2\sum_{j\neq l} \lambda_j\lambda_l = \frac{1}{2}C^2(\Psi). \tag{A17}$$

This inequality is tight, as $\ell_{\text{off,2-sec}} = \frac{1}{2}C^2(\Psi)$ in the Schmidt basis. Thus our proof is complete. ■

[1] E. Schmidt, Zur Theorie der linearen und nichtlinearen integralgleichungen, Math. Ann. **63**, 433 (1906).
[2] H. Everett III, "Relative state" formulation of quantum mechanics, Rev. Mod. Phys. **29**, 454 (1957).
[3] A. Ekert and P. L. Knight, Entangled quantum systems and the Schmidt decomposition, Am. J. Phys. **63**, 415 (1995).
[4] I. Bengtsson and K. Zyczkowski, *Geometry of Quantum States* (Cambridge University, Cambridge, England, 2006).
[5] M. M. Wolf, Quantum channels and operations guided tour, lecture notes, available at http://www-m5.ma.tum.de/foswiki/pub/M5/Allgemeines/MichaelWolf/QChannelLecture.pdf.
[6] In the case of pure states, the operator Schmidt decomposition essentially retrieves the pure-state decomposition; it is not difficult to see this by considering Eq. (4) and viewing (jk) as a single two-digit index that runs from 1 through $d_A d_B$, the dimension of an appropriate operator basis.
[7] M. A. Nielsen, C. M. Dawson, J. L. Dodd, A. Gilchrist, D. Mortimer, T. J. Osborne, M. J. Bremner, A. W. Harrow, and A. Hines, Quantum dynamics as a physical resource, Phys. Rev. A **67**, 052301 (2003).
[8] D. Cariello, Separability for weakly irreducible matrices, Quant. Inf. Comput. **14**, 1308 (2014).

[9] L. R. Tucker, Some mathematical notes on three-mode factor analysis, Psychometrika **31**, 279 (1966).
[10] H. Carteret, A. Higuchi, and A. Sudbery, Multipartite generalization of the Schmidt decomposition, J. Math. Phys. **41**, 7932 (2000).
[11] L. De Lathauwer, B. De Moor, and J. Vandewalle, A multilinear singular value decomposition, SIAM J. Matrix Anal. Appl. **21**, 1253 (2000).
[12] F. Sokoli and G. Alber, Generalized Schmidt decomposability and its relation to projective norms in multipartite entanglement, J. Phys. A: Math. Theor. **47**, 325301 (2014).
[13] A. Acín, A. Andrianov, L. Costa, E. Jané, J. I. Latorre, and R. Tarrach, Generalized Schmidt Decomposition and Classification of Three-Quantum-Bit States, Phys. Rev. Lett. **85**, 1560 (2000).
[14] T. Hiroshima and M. Hayashi, Finding a maximally correlated state: Simultaneous Schmidt decomposition of bipartite pure states, Phys. Rev. A **70**, 030302(R) (2004).
[15] U. Fano, Description of states in quantum mechanics by density matrix and operator techniques, Rev. Mod. Phys. **29**, 74 (1957).
[16] J. Schlienz and G. Mahler, Description of entanglement, Phys. Rev. A **52**, 4396 (1995).
[17] G. Mahler and V. A. Weberruß, *Quantum Networks*, 2nd ed. (Springer, Berlin, 2004).
[18] P. Badziag, C. Brukner, W. Laskowski, T. Paterek, and M. Zukowski, Experimentally Friendly Geometrical Criteria for Entanglement, Phys. Rev. Lett. **100**, 140403 (2008).
[19] C. Klöckl and M. Huber, Characterizing multipartite entanglement without shared reference frames, Phys. Rev. A **91**, 042339 (2015).
[20] M.-C. Tran, B. Dakić, F. Arnault, W. Laskowski, and T. Paterek, Quantum entanglement from random measurements, Phys. Rev. A **92**, 050301(R) (2015).
[21] F. Huber, O. Gühne, and J. Siewert, Absolutely Maximally Entangled States of Seven Qubits Do Not Exist, Phys. Rev. Lett. **118**, 200502 (2017).
[22] C. Eltschka and J. Siewert, Distribution of entanglement and correlations in all finite dimensions, Quantum **2**, 64 (2018).
[23] P. J. Appel, M. Huber, and C. Klöckl, Monogamy of correlations and entropy inequalities in the Bloch picture, J. Phys. Commun. (2020), doi:10.1088/2399-6528/ab6fb4.
[24] J. Preskill, Lecture notes on quantum computation, http://theory.caltech.edu/~preskill/ph229/.
[25] R. A. Horn and C. R. Johnson, *Topics in Matrix Analysis* (Cambridge University Press, Cambridge, 1994).
[26] Note that we call the terms in Eq. (15) sector "lengths" although, strictly speaking, these are squared Hilbert-Schmidt lengths of the corresponding operators. This terminology (introduced in Ref. [20]) is convenient and in general does not lead to confusion.
[27] P. Rungta, V. Buzek, C. M. Caves, M. Hillery, and G. J. Milburn, Universal state inversion and concurrence in arbitrary dimensions, Phys. Rev. A **64**, 042315 (2001).
[28] M. Huber (private communication).
[29] J. M. Steele, *The Cauchy Schwarz Master Class* (Cambridge University, Cambridge, England, 2004), Chap. 13.