

Broken symmetries in the entanglement of formation

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We compare some recent computations of the entanglement of formation in quantum information theory and of the entropy of a subalgebra in quantum ergodic theory. Both notions require optimization over decompositions of quantum states. We show that both functionals are strongly related for some highly symmetric density matrices. Indeed, for certain interesting regions the entanglement of formation can be expressed by the entropy of a commuting subalgebra, and the corresponding optimal decompositions can be obtained one from the other. We discuss the presence of broken symmetries in relation with the structure of the optimal decompositions. © 2003 American Institute of Physics.

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I. INTRODUCTION

Entanglement, always one of the most intriguing among quantum marvels, has lately become a powerful resource in prospective quantum information technologies;¹ measuring the entanglement content of states of multipartite quantum systems is thus of great practical importance. If a bipartite system $A+B$ is described by a density matrix ρ_{AB} , the so-called entanglement of formation² is measured by

$$E(\rho_{AB}) := \inf \left\{ \sum_j \lambda_j S(\text{Tr}_B \pi_j) : \rho_{AB} = \sum_j \lambda_j \pi_j \right\}. \quad (1)$$

In the above expression, $S(\rho) := -\text{Tr} \rho \log \rho$ denotes the von Neumann entropy of the state obtained by partial trace over B and the infimum is computed over all possible decompositions of ρ as convexly linear combinations, that is $\lambda_j > 0$, $\sum \lambda_j = 1$, of one-dimensional projections π_j of $A+B$. In the following we call such decompositions *extremal convex decompositions* of ρ to be distinguished from generic convex decompositions into mixed states.

When $\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|$, the entanglement of formation gives the asymptotic ratio between the number of singlet states necessary to construct $N \gg 1$ copies of ρ_{AB} .³ In the following, we will compare the entanglement of formation with a particular case of a more general quantity, the “entanglement with respect to a subalgebra” or “entanglement,” for short. This latter concept is related to the so-called “entropy of a subalgebra” \mathcal{A} contained in a reference algebra \mathcal{M} , relative to a state ρ on \mathcal{M} ,⁴

$$H_\rho(\mathcal{A}) := S(\rho \upharpoonright \mathcal{A}) - \inf \left\{ \sum_j \lambda_j S(\rho_j \upharpoonright \mathcal{A}) : \rho = \sum_j \lambda_j \rho_j \right\}. \quad (2)$$

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In the above expression, $S(\rho_j \upharpoonright \mathcal{A})$ is the von Neumann entropy of the state ρ_j restricted to the subalgebra \mathcal{A} and the infimum is calculated over all convexly linear decompositions of ρ into other states on \mathcal{M} . It plays a key role in extending the classical dynamical entropy of Kolmogorov to quantum systems.⁵⁻⁷ The entanglement of formation (1) can be considered a special case of (3), as explained in Remark 2.1.ii below.

We shall call “optimal” those decompositions achieving the extremum in (1) and (2). Calculating either $E(\rho_{AB})$ or $H_\rho(\mathcal{A})$ is particularly complicated. The problem has been completely solved for the entanglement of formation if $\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^2$,⁸ and for the entropy of a subalgebra if $\mathcal{M} = M_2(\mathbb{C})$.^{17,9,10} So far, all other available results concern states ρ_{AB} and ρ that are highly symmetric, isotropic in Ref. 11, respectively, permutation-invariant in Ref. 13.

In this paper we will discuss the previously mentioned results by comparing the two notions of entanglement sketched above. We show, that some of them are one-to-one related. To do so, we shall focus on the structure of optimal decompositions in relation to the symmetries existing in the problem and show possible ways of breaking them. These symmetries form a group G and leave invariant both the state ρ and, as a set, the subalgebra \mathcal{A} . Given extremal optimal decompositions, the G -orbits of each of their pure states consist of optimal decomposers, too. We will study the dependence of either entanglements upon the number of different orbits.¹²

II. ENTANGLEMENT

In the following, we shall consider quantum systems described by algebras of operators, \mathcal{M} , acting on finite or infinite dimensional Hilbert spaces \mathcal{H} , with states, $\mathcal{M} \ni X \mapsto \text{Tr}(\rho X)$, represented by density matrices which we shall denote by greek letters.

Definition 2.1: Given a finite dimensional subalgebra $\mathcal{A} \subseteq \mathcal{M}$, we define the entanglement of the state ρ with respect to \mathcal{A} by

$$E(\rho; \mathcal{M}, \mathcal{A}) := \inf \left\{ \sum_j \lambda_j S(\rho_j \upharpoonright \mathcal{A}) : \rho = \sum_j \lambda_j \rho_j \right\}, \quad (3)$$

where $\rho = \sum_j \lambda_j \rho_j$ runs through all convexly linear decompositions of ρ with states of \mathcal{M} , and $S(\rho_j \upharpoonright \mathcal{A})$ is the von Neumann entropy of the state ρ_j restricted to the subalgebra \mathcal{A} .

Remarks 2.1:

(i) The entanglement (3) is a convex functional over the states,

$$E\left(\sum_j \mu_j \rho_j; \mathcal{M}, \mathcal{A}\right) \leq \sum_j \mu_j E(\rho_j; \mathcal{M}, \mathcal{A}), \quad \sum_j \mu_j = 1, \quad \mu_j \geq 0. \quad (4)$$

This follows by choosing optimal decompositions for the ρ_j 's, which together provide a decomposition, not necessarily optimal, for $\sum_j \mu_j \rho_j$.

(ii) The entanglement of formation in equation (1) can be obtained from equation (3) as follows: set $\mathcal{M} = \mathcal{A} \otimes \mathcal{B}$, where \mathcal{A} and \mathcal{B} are the algebras of observables of the systems \mathcal{A} and \mathcal{B} . With $\rho = \rho_{AB}$ it turns out that $\rho_{AB} \mathcal{A} = \text{Tr}_B \rho_{AB}$.

(iii) The entanglement (3) is related with the entropy of a subalgebra (2) by

$$E(\rho_{AB}) = S(\rho_{AB} \upharpoonright \mathcal{A} \otimes \mathbf{1}_B) - H_{\rho_{AB}}(\mathcal{A} \otimes \mathbf{1}_B). \quad (5)$$

Indeed, as we shall see below in Proposition 2.1, the infimum is achieved at decompositions using pure states of \mathcal{M} only, and it enjoys some further remarkable properties.

The quantity in (5) and some techniques^{13,14} that were developed for computing (2), have recently been used to attack the question whether the entanglement of formation is additive.¹⁵ Among them, a useful result is contained in the following proposition. The idea is in Ref. 13 and, slightly extended, in Ref. 19. We include a proof for the benefit of the reader.

Proposition 2.1: If the algebra \mathcal{M} is finite dimensional, then

- (1) the entanglement $E(\rho; \mathcal{M}, \mathcal{A})$ is achieved at certain extremal convex decompositions $\rho = \sum_j \lambda_j \pi_j$, $\lambda_j > 0$ which saturate (3). Such decompositions are called *optimal*. Every pure state, π , which appears in at least one optimal decomposition of ρ is called ρ -*optimal* or an *optimal decomposer* of ρ .
- (2) For every ρ there is an optimal decomposition with a length not exceeding the linear dimension of \mathcal{M} .
- (3) The functional $E(\cdot; \mathcal{M}, \mathcal{A})$ is convexly linear on the convex hull $\mathcal{R}(\rho)$ of all ρ -optimal pure states: Let $\omega = \sum_i \alpha_i \pi_i$, $\alpha_i > 0$, $\sum_i \alpha_i = 1$ be any extremal convex decomposition where the π_i are some optimal decomposers of ρ . Then,

$$E(\omega; \mathcal{M}, \mathcal{A}) = \sum_i \alpha_i S(\pi_i \upharpoonright \mathcal{A}). \tag{6}$$

Proof: Any mixed state ρ can be decomposed and, since the von Neumann entropy is concave on convex combinations, mixed states cannot improve (3) with respect to pure states. If \mathcal{M} is d dimensional, compactness of the state space, extremality and compactness of the set of pure states ensure by a theorem of Caratheodory that we need not less than d and not more than d^2 decomposers.^{10,16} Because of convexity (4), the functional $E(\cdot; \mathcal{M}, \mathcal{A})$ is the supremum over affine functionals. Thus, for every ρ there are functionals ℓ such that $E(\rho; \mathcal{M}, \mathcal{A}) = \ell(\rho)$, while, on generic states σ , $E(\sigma; \mathcal{M}, \mathcal{A}) \geq \ell(\sigma)$. Given an optimal decomposition $\rho = \sum_j \lambda_j \pi_j$ it follows

$$E(\rho; \mathcal{M}, \mathcal{A}) = \sum_j \lambda_j E(\pi_j; \mathcal{M}, \mathcal{A}) \geq \sum_j \lambda_j \ell(\pi_j) = \ell(\rho) = E(\rho; \mathcal{M}, \mathcal{A}). \tag{7}$$

Since equality must hold in (7) and because $\lambda_j > 0$, while $E(\pi_j; \mathcal{M}, \mathcal{A}) \geq \ell(\rho)$ by assumption, we conclude $E(\pi_j; \mathcal{M}, \mathcal{A}) = \ell(\pi_j)$ for all j . With $\omega \in \mathcal{R}(\rho)$, let us now fix this affine functional ℓ and consider the extremal decomposition $\omega = \sum_k \alpha_k \pi'_k$ such that all the π'_k are optimal decomposers of ρ . By convexity and the preceding argument we deduce

$$E(\omega; \mathcal{M}, \mathcal{A}) \leq \sum_k \alpha_k E(\pi'_k; \mathcal{M}, \mathcal{A}) = \sum_k \alpha_k \ell(\pi'_k) = \ell(\omega). \tag{8}$$

However, $\ell(\omega) \leq E(\omega; \mathcal{M}, \mathcal{A})$ by our choice of ℓ , and equality holds in (8). Thus, $E(\cdot; \mathcal{M}, \mathcal{A})$ is convexly linear on $\mathcal{R}(\rho)$. ■

Definition 2.2: We shall call the convex hull $\mathcal{R}(\rho)$ of the optimal decomposers of ρ a *leaf* with respect to the entanglement $E(\rho; \mathcal{M}, \mathcal{A})$. Then, the state space appears as covered by leaves, and the entanglement itself is convexly linear above every leaf. That effect is referred to as the *roof property* of $E(\cdot; \mathcal{M}, \mathcal{A})$,¹⁰ i.e., $E(\cdot; \mathcal{M}, \mathcal{A})$ is a convex roof.

Definition 2.3: Given ρ on \mathcal{M} , we shall call a group G a symmetry group with respect to $E(\rho; \mathcal{M}, \mathcal{A})$, if for all $g \in G$ there exists a linear map $\gamma_g: \mathcal{M} \rightarrow \mathcal{M}$ such that the state and the subalgebra \mathcal{A} (as a set) are left invariant by γ_g , namely, $\gamma_g^*[\rho] = \rho$, where $\gamma_g^*[\rho](m) = \text{Tr}(\rho \gamma_g(m))$.

Proposition 2.2: If G is a symmetry group with respect to $E(\rho; \mathcal{M}, \mathcal{A})$, the leaf $\mathcal{R}(\rho)$ is G -invariant as a set. In particular, the action of G permutes the optimal decomposers of ρ .

Proof: Let $\rho = \sum_{j \in J} \lambda_j \rho_j$ be an optimal decomposition with respect to $E(\rho; \mathcal{M}, \mathcal{A})$. Then, since $\gamma_g^*[\rho] = \rho$ and $\gamma(\mathcal{A}) = \mathcal{A}$ for $g \in G$, the decomposition $\rho = \sum_{j \in J} \lambda_j \gamma_g^*(\rho_j)$ is also optimal. Therefore, its leaf $\mathcal{R}(\rho)$ must contain both the ρ_j 's and the $\gamma_g^*(\rho_j)$'s. ■

Based on the previous two propositions, the entropy $H_\rho(\mathcal{A})$ has explicitly been computed in the following cases:

Case 1: (Refs. 17, 9, 10) Let \mathcal{M} be the full 2×2 matrix algebra $M_2(\mathbf{C})$, \mathcal{A} the subalgebra of all 2×2 matrices diagonal with respect to a given basis $|1\rangle, |2\rangle$, and $\rho = \begin{pmatrix} a & b \\ b^* & 1-a \end{pmatrix}$, $0 \leq a \leq 1, |b|^2 \leq a(1-a)$, any density matrix.

Case 2: (Ref. 13) Let $\mathcal{M} = M_3(\mathbf{C})$, \mathcal{A} the subalgebra of all 3×3 diagonal matrices with respect to the basis $|1\rangle, |2\rangle, |3\rangle$ and

$$\rho(x) = \frac{1}{3} \begin{pmatrix} 1 & x & x \\ x & 1 & x \\ x & x & 1 \end{pmatrix}, \quad -1/2 \leq x \leq 1, \tag{9}$$

any density matrix invariant under the group of permutations of $\{1,2,3\}$.

For future comparison with the entanglement of formation of isotropic states of d -dimensional bipartite systems studied in Ref. 11, we fix an orthonormal basis $|j\rangle \in \mathbf{C}^d$ and consider the group G of permutations of $\{1,2,\dots,d\}$. It turns out that any G -invariant density matrix $\rho(x)$ over $\mathcal{M} = M_d(\mathbf{C})$ can be written as

$$\rho_F = \frac{1-F}{d-1} (\mathbf{1} - |\psi\rangle\langle\psi|) + F|\psi\rangle\langle\psi|, \tag{10}$$

where $|\psi\rangle = (1/\sqrt{d}) \sum_{j=1}^d |j\rangle$ and F is the fidelity parameter

$$0 \leq F := \langle\psi|\rho(x)|\psi\rangle = \frac{(d-1)x+1}{d-1} \leq 1. \tag{11}$$

Setting $s(t) := -t \log t$, we have

Case 1: For all ρ , the optimal decompositions are

$$\rho = \lambda |w_1\rangle\langle w_1| + (1-\lambda) |w_2\rangle\langle w_2|, \tag{12}$$

$$|w_1\rangle = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \quad |w_2\rangle = \begin{pmatrix} z_2^* \\ z_1^* \end{pmatrix}, \quad b = z_1 z_2^*, \tag{13}$$

$$|z_1|^2 = (1 + \sqrt{1-4|b|^2})/2 = 1 - |z_2|^2, \quad \lambda = \frac{1}{2} \left(1 + \frac{2a-1}{\sqrt{1-4|b|^2}} \right). \tag{14}$$

The corresponding entanglement is $E(\rho; M_2(\mathbf{C}), \mathcal{A}) = s(|z_1|^2) + s(|z_2|^2)$.

If $\rho = \rho_F$ is permutation-invariant, that is, if $a = 1/2$, $b = x/2$, $F = (1+x)/2$, the entanglement reads

$$E(\rho_F; M_2(\mathbf{C}), \mathcal{A}) = s\left(\frac{1+2\sqrt{F(1-F)}}{2}\right) + s\left(\frac{1-2\sqrt{F(1-F)}}{2}\right). \tag{15}$$

Case 2: Given the group G of permutations of $\{1,2,3\}$, let V, V^2 implement unitarily the subgroup G_0 of cyclic permutations. Then, any G -invariant state ρ_F can be written

$$\rho_F = \frac{1}{3} |w\rangle\langle w| + \frac{1}{3} V |w\rangle\langle w| V^{-1} + \frac{1}{3} V^2 |w\rangle\langle w| V^{-2}, \tag{16}$$

where

$$|w\rangle = \frac{1}{3} \begin{pmatrix} a+2b \cos \theta \\ a-2b \cos(\theta-\pi/3) \\ a-2b \cos(\theta+\pi/3) \end{pmatrix}, \quad a = \sqrt{3F}, \quad b = \sqrt{\frac{3}{2}(1-F)}. \tag{17}$$

The structure of optimal decompositions depends on the convexity of

$$\mathcal{S}(F) := \min_{\theta \in [0, 2\pi]} \sum_{j=1}^3 s(|w_j(F; \theta)|^2). \tag{18}$$

For $F \geq F^* := (2x^* + 1)/3$, $x^* = -0.415\,023\,4$, the minimum is achieved at a single extremal G_0 -orbit generated by the vectors

$$|w\rangle = \frac{1}{3} \begin{pmatrix} a + 2b \\ a - b \\ a - b \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{F} + \sqrt{2(1-F)} \\ \sqrt{F} - \sqrt{(1-F)/2} \\ \sqrt{F} - \sqrt{(1-F)/2} \end{pmatrix}. \tag{19}$$

For each $0 < F < F^*$, there are two different orbit-generating vectors, $|w_{\pm}(F)\rangle$, whose G_0 -orbits provide different optimal decomposers for (18), and which form together one orbit of the full permutation group G . They are

$$|w_{\pm}(F)\rangle = \frac{1}{3} \begin{pmatrix} a + 2b \cos \alpha_F \\ a - 2b \cos(\pi/3 \mp \alpha_F) \\ a - 2b \cos(\pi/3 \pm \alpha_F) \end{pmatrix}, \tag{20}$$

where the angle α_F varies with $0 < F < F^*$.

Finally, for $F = 0$, $\alpha_F = -\pi/6$, the minimum is achieved again at a single G -orbit containing the vector, $|w_0\rangle = (1/\sqrt{2})(1, 0, -1)$. As the 6 vectors coincide pairwise up to a sign, the states form a single optimal decomposition of length 3.

In Ref. 13, it is shown that the above vectors give optimal decompositions as long as the function $\mathcal{S}(F)$ is convex. Numerically, this is the case for all $F \leq 8/9$. The corresponding entanglement is

$$E(\rho_F; M_3(\mathbf{C}), \mathcal{A}) = s\left(\frac{2 - F + 2\sqrt{2F(1-F)}}{3}\right) + 2s\left(\frac{1 + F - 2\sqrt{2F(1-F)}}{6}\right) \tag{21}$$

for fidelities $F^* \leq F \leq 8/9$. For $F = 0$ the entanglement equals $\log 2$. We have only numerical results within the interval $0 < F < F^*$,¹⁴ reflecting that the exact dependence of the angle α_F in (20) as a function of F is unknown.

Remark 2.2: Permutation-invariant states as in (10) can be written as averages over the unitaries U_{π} implementing the permutation group G ,

$$\rho_F = \frac{1}{d!} \sum_{\pi} U_{\pi}^{-1} |\phi\rangle\langle\phi| U_{\pi}, \tag{22}$$

if and only if $|\langle\psi|\phi\rangle|^2 = F$, where $|\psi\rangle$ is the vector in (11). Necessity comes from the fact that $U_{\pi}|\psi\rangle = |\psi\rangle$. Sufficiency: The identity $\mathbf{1}$ and $|\psi\rangle\langle\psi|$ form a basis for all possible contributions to the averages (22).

In view of the structure of the optimal decomposers discussed above, we introduce a notion of regularity with respect to a subgroup of a symmetry group, as follows:

Definition 2.4: Given a symmetry group G with respect to $E(\rho; \mathcal{M}, \mathcal{A})$, we shall call a leaf $\mathcal{R}(\rho)$ regular of order n with respect to a subgroup $H \subset G$, if there exists n pure states $\bar{\rho}_j \in \mathcal{R}(\rho)$ such that $\gamma_h^*[\bar{\rho}_j] = \bar{\rho}_j$ for all $h \in H$, whereas the convex span of the orbits $\{\gamma_g^*[\bar{\rho}_j]\}_{g \in G}$ is the whole of $\mathcal{R}(\rho)$.

We illustrate the previous definitions with some examples.

Example 2.1: Let \mathcal{M} be a full $d \times d$ matrix algebra on \mathbf{C}^d and $\mathcal{A} \subset \mathcal{M}$ diagonal with respect to a chosen orthonormal basis $\{|j\rangle\}_{j=1}^d$ in \mathbf{C}^d . Let ρ be a symmetric density matrix, $\langle j|\rho|k\rangle = \langle k|\rho|j\rangle$. Then, with respect to the chosen representation, the transposition \mathcal{T} respects both the state and the subalgebra \mathcal{A} . Also, $\mathcal{R}(\rho)$ is regular with respect to $G = H = \{\text{id}, \mathcal{T}\}$, the order of

regularity depending on the state ρ . In fact, let $\pi = |\psi\rangle\langle\psi| \in \mathcal{R}(\rho)$, then, because of Proposition 2.2, $\mathcal{T}(\pi) = \pi' = |\psi'\rangle\langle\psi'| \in \mathcal{R}(\rho)$, too. If $\pi \neq \pi'$, we may consider the state $\omega = \pi/2 + \pi'/2$, which, by Proposition 2.1, is already optimally decomposed. Also,

$$E(\omega; \mathcal{M}, \mathcal{A}) = S(\pi \upharpoonright \mathcal{A}) = S(\omega \upharpoonright \mathcal{A}). \quad (23)$$

Instead, the decomposition

$$\omega = \frac{1 + \operatorname{Re}(\langle\psi|\psi'\rangle)}{2} \pi_+ + \frac{1 - \operatorname{Re}(\langle\psi|\psi'\rangle)}{2} \pi_-, \quad (24)$$

where

$$\pi_{\pm} = \frac{|\psi \pm \psi'\rangle\langle\psi \pm \psi'|}{2(1 \pm \operatorname{Re}(\langle\psi|\psi'\rangle))} \quad (25)$$

need not be optimal. However, the concavity of the von Neumann entropy yields

$$E(\omega; \mathcal{M}, \mathcal{A}) \leq \frac{1 + \operatorname{Re}(\langle\psi|\psi'\rangle)}{2} S(\pi_+ \upharpoonright \mathcal{A}) + \frac{1 - \operatorname{Re}(\langle\psi|\psi'\rangle)}{2} S(\pi_- \upharpoonright \mathcal{A}) \leq S(\omega \upharpoonright \mathcal{A}). \quad (26)$$

It thus follows from (23) that $\pi \upharpoonright \mathcal{A} = \pi_{\pm} \upharpoonright \mathcal{A}$, whence the components $\psi(i)$, $\psi'(i)$ of ψ and ψ' must coincide apart from an overall phase. Thus, $\pi = \pi'$ and the \mathcal{T} -symmetry cannot be broken.

Example 2.2: Let $\mathcal{M} = \mathcal{A} \otimes \mathcal{B}$, with \mathcal{A} and \mathcal{B} isomorphic and $\sigma: \mathcal{A} \rightarrow \mathcal{B}$ the algebraic exchange of the two of them. If ρ is a state on \mathcal{M} such that $\rho \circ (\sigma^{-1} \otimes \sigma) = \rho$, in general, $\sigma^{-1} \otimes \sigma$ does not belong to any subgroup of regularity of ρ ; indeed, if \mathcal{A} (and thus \mathcal{B}) is a d -dimensional matrix algebra and $\{|\ell\rangle\}$ is an orthonormal basis in the corresponding Hilbert space $\mathcal{H}_{\mathcal{A}}$ (and thus also in $\mathcal{H}_{\mathcal{B}}$), the density matrix

$$\rho_{AB} := \frac{1}{2} |1\rangle\langle 1| \otimes |2\rangle\langle 2| + \frac{1}{2} |2\rangle\langle 2| \otimes |1\rangle\langle 1|, \quad (27)$$

is such that $\operatorname{Tr}(\rho(\sigma^{-1} \otimes \sigma)(X \otimes Y)) = \operatorname{Tr}(\rho(X \otimes Y))$. Also, ρ_{AB} is already optimally decomposed, $E(\rho_{AB}; \mathcal{A}, \mathcal{M}) = 0$ is achieved with the decomposers $|1\rangle\langle 1| \otimes |2\rangle\langle 2|$ and $|2\rangle\langle 2| \otimes |1\rangle\langle 1|$, which, however, are not invariant under $\sigma^{-1} \otimes \sigma$.

Example 2.3: Let $\mathcal{M} = \mathcal{A} \otimes \mathcal{B}$, with \mathcal{A} and \mathcal{B} both $d \times d$ full matrix algebras. We fix the same orthonormal basis $\{|\ell\rangle\}$ in both Hilbert spaces $\mathcal{H}_{\mathcal{A}, \mathcal{B}}$ and consider the one-parameter group U of unitaries

$$U_t := \sum_{j,k} e^{it(h_j - h_k)} |j\rangle\langle j| \otimes |k\rangle\langle k|. \quad (28)$$

The density matrix $\rho_{AB} := \sum_{j,k} R_{jk} |j\rangle\langle k| \otimes |j\rangle\langle k|$, $R = [R_{jk}] \geq 0$, $\operatorname{Tr} R = 1$, is U -invariant; moreover, $\sqrt{\rho_{AB}} = \sum_{j,k} (\sqrt{R})_{jk} |j\rangle\langle k| \otimes |j\rangle\langle k|$, so that the operators $\sqrt{\rho_{AB}} M \sqrt{\rho_{AB}}$, $M \in \mathcal{M}$, have the same matrix structure as ρ_{AB} . Choosing positive $M_j \geq 0$, $j \in J$, such that $\sum_{j \in J} M_j = 1$, ρ_{AB} decomposes into

$$\rho_{AB} = \sum_{j \in J} (\operatorname{Tr}(\rho_{AB} M_j)) \frac{\sqrt{\rho_{AB}} M_j \sqrt{\rho_{AB}}}{\operatorname{Tr}(\rho_{AB} M_j)}. \quad (29)$$

Since it is also true that every mixed state ρ on \mathcal{M} can be written as in (29) by means of a suitable positive M_j , (29) indeed exhausts all possible decompositions of ρ_{AB} . Thus, the decomposers π_j of ρ_{AB} which are optimal with respect to $E(\rho_{AB}; \mathcal{M}, \mathcal{A})$, have the same structure of ρ_{AB} and are

then U -invariant. Hence, the group U is a group of symmetries of ρ_{AB} with respect to entanglement and the leaf $\mathcal{R}(\rho_{AB})$ is regular with respect to $H \equiv U$, its order depending on which further symmetries are enjoyed by ρ_{AB} .

Example 2.4: Let $\mathcal{M} = M_2(\mathbf{C})$, \mathcal{A} as in Case 1, and ρ_F a permutation-invariant state. The leaf $\mathcal{R}(\rho_F)$ is the orbit of the group G of permutations of $\{1,2\}$. This follows from the form of the optimal vectors (12) in such a case: $|w_1\rangle = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$, $|w_2\rangle = \begin{pmatrix} z_2 \\ z_1 \end{pmatrix}$, with $z_{1,2} = \sqrt{1/2(1 \pm 2\sqrt{F(1-F)})}$. It is regular of order 1 with respect to rotations with elements from \mathcal{A} .

Example 2.5: Let $\mathcal{M} = M_3(\mathbf{C})$ and ρ_F a permutation-invariant state. Then, for $F^* \leq F$ and F belonging to the convexity region of $\mathcal{S}(F)$ in (18), the structure of the optimal vectors (19) ensures that the leaf $\mathcal{R}(\rho_F)$ is regular of order 1 for the subgroup H of permutations $\{2,3\} \mapsto \{3,2\}$. However, at the point $F = F^*$ such a H -invariant vector bifurcates into the two optimal ones (20). Thus regularity with respect to the subgroup H is broken and remains broken for $0 < F < F^*$. At $F = 0$ optimal vector states of different G_0 orbits degenerate pairwise into a single one, and one of them is H -invariant, while the corresponding vector changes its sign.

In the last two examples, for all F when $d = 2$, and for F greater than the bifurcation values F^* in the convexity region of $\mathcal{S}(F)$ in (18), when $d = 3$, the leaf $\mathcal{R}(\rho_F)$ of a permutation-invariant ρ_F is generated by the orbit under the subgroup G_0 of cyclic permutations $V^j|w\rangle$, $j = 0, 1, 2$. The vector $|w\rangle$ is invariant under a unique transposition out of G . This structure is indeed more general as will be shown in the next two propositions.

Proposition 2.3: Let $\mathcal{A} \subset \mathcal{M} = M_d(\mathbf{C})$ be chosen as in Example 2.1 and the density matrix ρ_F be invariant with respect to the permutation group G . If the leaf $\mathcal{R}(\rho_F)$ with respect to \mathcal{A} is generated by exactly one G_0 -orbit of a normalized vector state $|w\rangle \in \mathbf{C}^d$, with $G_0 \subset G$ the subgroup of cyclic permutations, then the entanglement is

$$E(\rho_F; M_d(\mathbf{C}, \mathcal{A})) = s(p_F) + (d-1)s\left(\frac{1-p_F}{d-1}\right), \tag{30}$$

$$p_F := \frac{|\sqrt{F} + \sqrt{(d-1)(1-F)}|^2}{d}. \tag{31}$$

Remarks 2.3:

(i) The assumption of the previous proposition amounts to ask $\mathcal{R}(\rho_F)$ to be regular of order 1 with respect to the subgroup $H \subset G$ of permutations on $\{2, 3, \dots, d\}$. Indeed, the leaf is G -invariant, so that the d states $|\phi_j\rangle = V^j|w\rangle$, $j = 0, 1, \dots, d-1$, obtained via cyclic permutations, must be invariant under the remaining $(d-1)!$ permutations. This is possible only if $d-1$ of the d components of the optimal vector $|w\rangle$ are equal.

(ii) If $|w\rangle$ has three different components, then the decompositions (22) contain at least $d(d-1)$ different terms.

(iii) In Sec. III we will show that, upon identification of p_F with the quantity $\gamma(F)$ in Ref. 11, the entanglement of formation calculated there is given by (31) and (30) in a range $F^{**} \geq F > 1/d$. The upper limit F^{**} is a particular bifurcation point which was discovered in Ref. 11 and that will be reinterpreted accordingly within the framework of this work.

Proof: By hypothesis, $\rho_F = 1/d \sum_{j=0}^{d-1} V^j|w\rangle\langle w|V^{-j}$ is an optimal decomposition with entanglement

$$E(\rho_F; M_d(\mathbf{C}), \mathcal{A}) = \sum_{j=1}^d s(|\langle j|w\rangle|^2). \tag{32}$$

Also, taking into account Remarks 2.2 and 2.3, and decomposing

$$|w\rangle = \sqrt{F}|\psi\rangle + \varepsilon\sqrt{1-F}|w_1^\perp\rangle = \alpha|1\rangle + \beta\sum_{j=2}^d |j\rangle,$$

where ε is a pure phase, it follows that $|w_1^\perp\rangle = (\sqrt{d}|1\rangle - |\psi\rangle)/\sqrt{d-1}$ and

$$|w\rangle = \frac{1}{\sqrt{d}} \left[(\sqrt{F} + \varepsilon \sqrt{(1-F)(d-1)})|1\rangle + \left(\sqrt{F} - \varepsilon \sqrt{\frac{1-F}{d-1}} \right) \sum_{j=2}^d |j\rangle \right].$$

With $\xi := 2 \operatorname{Re}(\varepsilon)$, the right-hand side of (32) reads

$$\begin{aligned} \mathcal{S}(\xi) &= s(p(\xi)) + (d-1)s\left(\frac{1-p(\xi)}{d-1}\right), \\ p(\xi) &= \frac{F + (1-F)(d-1) + \xi \sqrt{F(1-F)(d-1)}}{d}. \end{aligned}$$

It achieves its minimum at the maximum value of p that is for $\varepsilon = 1$, from which the result follows. Indeed, as we show below, $|w\rangle$ must be real. If remark 2.3(i) applies we always get a local extremum. Either by direct calculation or relying on Ref. 13 one concludes $\varepsilon = 1$. ■

We now relax the hypothesis of the previous proposition and allow for more than one G_0 -orbit to be optimal for the entanglement of ρ_F with respect to the subalgebra \mathcal{A} , that is we allow the leaf $\mathcal{R}(\rho_F)$ to be generated by more than one G_0 -orbit.

Proposition 2.4: Let $\mathcal{A} \subset \mathcal{M} = M_d(\mathbf{C})$ be chosen as in Example 2.1. If the density matrix ρ_F is invariant with respect to the permutation group G and its entanglement with respect to \mathcal{A} can be achieved at an optimal decomposition consisting of one G_0 -orbit of normalized vector states $|w\rangle \in \mathbf{C}^d$, with $G_0 \subset G$ the subgroup of cyclic permutations, then we have three possibilities:

- (1) $|w\rangle = 1/\sqrt{d} \sum_{k=1}^d |k\rangle$ in which case $F = 1$ and $\rho_F = |\psi\rangle\langle\psi|$;
- (2) $|w\rangle$ is real with 1 component equal to a_1 and $d-1$ real components all equal to $a_2 \neq a_1$;
- (3) $|w\rangle$ is real with 2 components $a_1 \neq a_3$ and $d-2$ components all equal to a_3 different from both a_1 and a_2 .

To prove the result we need a preliminary

Lemma 2.1: The vector $|w\rangle$ whose G_0 -orbit is optimal can be chosen real.

Proof: Let $v_k, k = 1, 2, \dots, d$, be the components of $|w\rangle$ with respect to the chosen orthonormal basis $\{|k\rangle\}$ and $|\psi\rangle = (1/\sqrt{d}) \sum_{k=1}^d |k\rangle$. The assumption is that $\rho_F = 1/d \sum_{j=0}^{d-1} V^j |w\rangle\langle w| V^{-j}$; from normalization it follows that the components of $|w\rangle$ must satisfy

$$\sum_{k=1}^d |w_k|^2 = 1, \quad \left| \sum_{k=1}^d w_k \right|^2 = 1 - \sum_{\ell \neq k=1}^d w_\ell^* w_j = dF. \tag{33}$$

Further, in order to implement optimality and achieve $E(\rho_F; \mathcal{M}, \mathcal{A})$, we minimize

$$\mathcal{S}(w, \lambda, \mu) := - \sum_{k=1}^d |w_k|^2 \log |w_k|^2 + \lambda \sum_{k=1}^d |w_k|^2 + \mu \sum_{\ell \neq k} w_\ell w_k^*, \tag{34}$$

with Lagrange multipliers λ, μ . Setting $v := \sum_{k=1}^d w_k = \sqrt{dF} e^{i\theta}$, equating to zero the derivative of (34) with respect to w_j and multiplying by w_j we get

$$-|w_j|^2 \log |w_j|^2 + (\lambda - 1)|w_k|^2 + \mu(v^* w_j - |w_j|^2) = 0.$$

Therefore, the quantity $v^* w_j \mu$ and thus, after summing over j , also μ , must be real, whence, necessarily $w_j = e^{i\theta} v_j$, with $v_j \in \mathbf{R}$, for all j . The result follows by eliminating the overall phase. ■

Proof: (Proposition 2.4) According to the previous Lemma, we choose $|w\rangle$ real and proceed to minimize

$$\mathcal{S}(w, \lambda, \mu) := - \sum_{k=1}^d w_k^2 \log w_k^2 + \lambda \sum_{k=1}^d w_k^2 + \mu \sum_{k=1}^d w_k. \tag{35}$$

Because of convexity, the function $g(x) := -x \log x^2$ intersects the straight line $f(x) := 2(1 - \lambda)x - \mu$ in at most three points on $[-1, 1]$. Therefore, the d solutions to

$$-2w_k \log w_k^2 - 2w_k + 2\lambda w_k + \mu = 0,$$

can have at most three different real values, $a_i, i = 1, 2, 3$. We denote by n_i the number of times they appear among the components and consider the functional

$$\mathcal{S}(\vec{a}; \vec{n}; \lambda, \mu, \nu) := - \sum_{i=1}^3 n_i a_i^2 \log a_i^2 + \lambda \sum_{i=1}^3 n_i a_i^2 + \mu \sum_{i=1}^3 n_i a_i, \tag{36}$$

where we treat the n_i 's as continuous variables constrained by $n_1 + n_2 + n_3 = d$. Minimizing (36) yields the following equations:

$$n_i(a_i \log a_i^2 + a_i - \lambda a_i - \mu) = 0, \quad i = 1, 2, 3, \tag{37}$$

$$-a_i^2 \log a_i^2 + \lambda a_i^2 + \mu a_i + \nu, \quad i = 1, 2, 3. \tag{38}$$

It follows that, if $n_i > 0, i = 1, 2, 3$, then $\sum_{i=1}^3 (\mu a_i + 2\nu + 2a_i^2) = 0, i = 1, 2, 3$, and thus $a = b = c$. This case corresponds to $\rho_{F=1} = |\psi\rangle\langle\psi|$, a pure state, with null entanglement with respect to \mathcal{A} . Therefore, if there are three different intersections, the minimum entanglement is reached at the boundary values of $n_i, i = 1, 2, 3$, that is, without loss of generality, at $n_1 = n_2 = 1$ and $n_3 = d - 2$. If there are two intersections, that is, if, without loss of generality, $n_3 = 0$ and $a_1 \neq a_2 = a_3$, then, from (37) and (38), we calculate $\mu = -2(a_1 + a_2), \mu = a_1 a_2$ and deduce the equality

$$a_1^2 - a_2^2 + a_1 a_2 \log \frac{a_2^2}{a_1^2} = 0.$$

For fixed a_1 , because of their convexity properties, the two functions $f(x) := \log(a_1^2/x^2)$ and $g(x) := (a_1/x) - (x/a_1)$ intersect at $x = a_1$, but, at no other points. Therefore, the entanglement is again minimal at the boundary, that is at, say $n_1 = 1$ and $n_2 = d - 1$. ■

Remark 2.4: Lagrange multipliers have been used in Ref. 11 in order to calculate the entanglement of formation of isotropic states of bipartite quantum systems, where it is shown that, when $F > 1/d$, the optimal decomposers have only two different components. We shall relate those results to ours in the following section, where we also discuss the fact, discovered in Ref. 11, stating there is a bifurcation point F^{**} such that the entanglement of formation is linear in F between F^{**} and $F = 1$.

Proposition 2.4 shows that when the vector $|w\rangle$ has only two different components, then we reduce to the case discussed in Proposition 2.3. Instead, when $|w\rangle$ has three different components, which is possible in a range of values of F , then we have more than one optimal decomposition. If $d = 3$ one gets at least two. Notice that these results are obtained under the hypothesis that G_0 -orbits of vectors $|w\rangle$ provide optimal decompositions for the entanglement of ρ_F with respect to the subalgebra \mathcal{A} .

This fact is linked to the convexity of the function (18), which, as observed in the discussion of Case 2, fails in a neighborhood of $F = 1$: If $F \geq F^{**}$ one needs two orbits: the optimal orbit for $F = F^{**}$ and the singlet for $F = 1$, just as observed in Ref. 11. Consequently, for $F^{**} < F < 1$ no G_0 -orbits can be optimal.

III. ENTANGLEMENT AND ENTANGLEMENT OF FORMATION

In this section we establish a one-to-one correspondence between the results of the previous section, in particular proposition 2.3, and the entanglement of formation of highly symmetric states as examined in Ref. 11. This concerns mainly the region $(1/d) \leq F$. From Ref. 11 we learned the existence of the bifurcation point F^{**} . On the other hand, our results in the region $(1/d) < F \leq F^{**}$ can be converted into those found by Terhal and Volbrecht. Indeed, the value of the entanglement of formation will be proved to be just (30).

To this end we consider the tensor product $\mathcal{M} := \mathcal{A} \otimes \mathcal{B}$ of the full $d \times d$ matrix algebra, denoted by \mathcal{A} , with a copy, \mathcal{B} , of itself. We fix an orthonormal basis $\{|j\rangle\}$ of \mathbf{C}^d and given any density matrix, that is a state on \mathcal{A} ,

$$\rho_A = \sum_{j,k} R_{jk} |j\rangle\langle k|, \quad R = [R_{jk}] \geq 0, \quad \text{Tr } R = 1, \quad (39)$$

we embed it as $D[\rho_A]$ into the state space of \mathcal{M} according to the following:

Definition 3.1: Let D be the linear map associating matrix units $|j\rangle\langle k|$ of \mathcal{A} with matrix units $\{|j\rangle\langle k| \otimes |j\rangle\langle k|\}$ of \mathcal{M} . We shall refer to it as the *doubling map*. It transforms states ρ_A on \mathcal{A} into states on $\mathcal{M} = \mathcal{A} \otimes \mathcal{B}$ of the form

$$\rho_A \mapsto D[\rho_A] := \sum_{j,k} R_{jk} |j\rangle\langle k| \otimes |j\rangle\langle k|. \quad (40)$$

Remark 3.1: This yields the class of density matrices in Example 2.3, which we shall refer to as diagonal class (with respect to the chosen basis). On the given diagonal class the doubling map can be inverted

$$D^{-1}: \rho_{AB} = \sum_{j,k} R_{j,k} |j\rangle\langle k| \otimes |j\rangle\langle k| \mapsto \rho_A = \sum_{j,k} R_{j,k} |j\rangle\langle k|. \quad (41)$$

The argument developed in Example 2.3 ensures that decompositions of ρ_A can be mapped onto decompositions of $D[\rho_A]$. Vice versa, decompositions of ρ_{AB} provide decompositions for the diagonal class of ρ_A by applying D^{-1} . Moreover, if $\mathcal{A}_0 \subset \mathcal{A}$ denotes the subalgebra of diagonal matrices in the given, fixed representation, then $S(\rho \upharpoonright \mathcal{A}_0) = S(D[\rho_A] \upharpoonright \mathcal{A})$. Therefore: *The entanglement is preserved by D* , in the sense that

$$E(\rho_A; \mathcal{A}, \mathcal{A}_0) = E(D[\rho_A]; \mathcal{A} \otimes \mathcal{B}, \mathcal{A}). \quad (42)$$

In Ref. 11 the entanglement of formation has been calculated for the isotropic states

$$\omega_F = \frac{1-F}{d^2-1} (\mathbf{1}_{AB} - |\Psi\rangle\langle\Psi|) + F |\Psi\rangle\langle\Psi|. \quad (43)$$

In the above expression $\mathbf{1}_{AB}$ is the identity for the algebra $\mathcal{A} \otimes \mathcal{B}$ and

$$|\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^d |j\rangle \otimes |j\rangle. \quad (44)$$

Remark 3.2: The isotropic states are invariant under the group \mathcal{G} of all unitaries of the form $U \otimes \tilde{U}$ where $\langle a|U|b\rangle = \langle a|\tilde{U}|b\rangle^*$,

$$U \otimes \tilde{U} \omega_F U^{-1} \otimes \tilde{U}^{-1} = \omega_F. \quad (45)$$

As in Remark 2.2, it follows that ω_F can be expressed as the following average with respect to the Haar measure $d_G U$,

$$\omega_F = \int_G d_G U U \otimes \tilde{U} |\Phi\rangle\langle\Phi| U^{-1} \otimes \tilde{U}^{-1}, \tag{46}$$

if and only if $F = \langle\Psi|\omega_F|\Psi\rangle = |\langle\Psi|\Phi\rangle|^2$.

We compare the isotropic state ω_F with the doubling of ρ_F in (10),

$$\begin{aligned} D[\rho_F] &= \frac{1-F}{d-1} (D[\mathbf{1}_A] - D[|\psi\rangle\langle\psi|]) + FD[|\psi\rangle\langle\psi|] \\ &= \frac{1-F}{d-1} \left(\sum_{j=1}^d |j\rangle\langle j| \otimes |j\rangle\langle j| - |\Psi\rangle\langle\Psi| \right) + F|\Psi\rangle\langle\Psi|. \end{aligned} \tag{47}$$

Proposition 3.1: Let $F > 1/d$ and consider the decomposition

$$\omega_F = \frac{1}{d!} \sum_{\pi} U_{\pi}^{-1} \otimes U_{\pi}^{-1} |\Phi\rangle\langle\Phi| U_{\pi} \otimes U_{\pi}$$

by means of the unitaries U_{π} that implement the permutation group G . If the latter is optimal for the entanglement of formation $E(\omega_F)$ with $|\Phi\rangle\langle\Phi|$ in the diagonal space, then $E(\omega_F) = E(\rho_F, \mathcal{A}, \mathcal{A}_0)$.

Proof: The $d!$ unitaries U_{π} form a subgroup $G \otimes G$ of the group of unitaries in Remark 3.2; they implement the permutation of the chosen basis $\{|j\rangle \otimes |j\rangle\}$ of the diagonal space. Then, $\langle\Psi|\omega_F|\Psi\rangle = \langle\Psi|D[\rho_F]|\Psi\rangle = F$ and

$$D[\rho_F] = \frac{1}{d!} \sum_{\pi} U_{\pi}^{-1} \otimes U_{\pi}^{-1} |\Phi\rangle\langle\Phi| U_{\pi} \otimes U_{\pi}.$$

If $|\Phi\rangle\langle\Phi|$ is optimal for ω_F , it turns out from Proposition 2.2 that the decomposeres $U \otimes \tilde{U} |\Phi\rangle\langle\Phi| U^{-1} \otimes \tilde{U}^{-1}$ are optimal, too. Thus the result follows from Proposition 2.1. ■

Remarks 3.3:

- (i) If $F > 1/d$ the isotropic state ω_F is entangled. When $F \leq 1/d$ it becomes separable. There exist several proofs of this fact, e.g., Ref. 18.
- (ii) In view of Remark 2.3(ii), the previous proposition establishes a link between our results and those of Ref. 11. In Ref. 11 a new symmetry breaking bifurcation point was observed at $F = 8/9$ when $d = 3$. The doubling map makes it correspond to a bifurcation point within case 2 of the previous section at the same value of F . The numerical analysis in Ref. 14 missed it, the needed accuracy being of the order of 10^{-4} . In both cases the leaves $\mathcal{R}(\omega_F)$, respectively, $\mathcal{R}(\rho_F)$, are identical for all F within $F^{**} = 8/9 < F < 1$. This unique leaf is generated by the optimal decompositions of $\omega_{8/9}$ which form one orbit, and by the pure state ω_1 given by (44). The same is true of $\rho_{8/9}$ and ρ_1 . The latter orbits are singlets.
- (iii) The entanglement of ρ_1 and $\rho_{8/9}$ that generate the leaf discussed in the previous remark do not coincide,¹⁹

$$E(\rho_1; \mathcal{M}, \mathcal{A}) = \ln 3, \quad E(\rho_{8/9}; \mathcal{M}, \mathcal{A}) = \ln 3 - \frac{1}{3} \ln 2. \tag{48}$$

We shall now relate the remark above to another observation which again relates entanglement of different algebras with one another.

From Case 1 in Sec. II, we know that vectors of the form $\binom{x}{y}$ and $\binom{y}{x}$, with $x^2 + y^2 = 1$ generate the leaf of some state ρ_2 on $M_2(\mathbb{C})$. These two-dimensional vectors can be embedded in \mathbb{C}^3 as follows:

$$|w_1\rangle = \begin{pmatrix} x \\ y/\sqrt{2} \\ y/\sqrt{2} \end{pmatrix}, \quad |w_2\rangle = \begin{pmatrix} y \\ x/\sqrt{2} \\ x/\sqrt{2} \end{pmatrix}. \tag{49}$$

With them we construct the density matrix in $M_3(\mathbf{C})$ of the form

$$\tilde{\rho}_3 = \lambda |w_1\rangle\langle w_1| + (1-\lambda) |w_2\rangle\langle w_2| = \begin{pmatrix} a & b & b \\ b & c & c \\ b & c & c \end{pmatrix}. \tag{50}$$

It is easy to check that powers of $\tilde{\rho}_3$ have the same structure which is thus inherited by $\sqrt{\tilde{\rho}_3}$. It thus follows that

$$\sqrt{\tilde{\rho}_3}|\phi\rangle = \begin{pmatrix} u \\ v \\ v \end{pmatrix}$$

for any $|\phi\rangle$. The discussion of Example 2.3 assures that the optimal decomposers of $\tilde{\rho}_3$ with respect to the entanglement $E(\tilde{\rho}; M_3(\mathbf{C}), \mathcal{A}_3)$, with \mathcal{A}_3 the maximally Abelian subalgebra in the chosen representation, have again the same form. But then, $\binom{x}{y}$ and $\binom{y}{x}$ being optimal with respect to $E(\rho_2; M_2(\mathbf{C}), \mathcal{A}_2)$, (50) is itself an optimal decomposition of $\tilde{\rho}_3$ with respect to $E(\tilde{\rho}_3; M_3(\mathbf{C}), \mathcal{A}_3)$.

According to the discussion at the beginning of this section, it also follows that the doubling map,

$$|w_1\rangle \mapsto |W_1\rangle = x|1\rangle \otimes |1\rangle + \frac{y}{\sqrt{2}}(|2\rangle \otimes |2\rangle + |3\rangle \otimes |3\rangle), \tag{51}$$

$$|w_2\rangle \mapsto |W_2\rangle = y|1\rangle \otimes |1\rangle + \frac{x}{\sqrt{2}}(|2\rangle \otimes |2\rangle + |3\rangle \otimes |3\rangle), \tag{52}$$

provides optimal decomposers, too. In particular, for given x, y on the unit circle the pure states $|W_j\rangle\langle W_j|$, $j=1,2$, generate a leaf of the entanglement of formation functional on which it is convexly linear.

Moreover, for $x = 1/\sqrt{3}$ and $y = \sqrt{2/3}$, we get $|W_1\rangle = |\Psi\rangle$, with fidelity $F = |\langle \Psi | W_1 \rangle|^2 = 1$, and $|W_2\rangle = |\Phi_{8/9}\rangle$ with fidelity $F = |\langle \Psi | W_2 \rangle|^2 = 8/9$, indicating a reason for the bifurcation value $F = 8/9$.

One observes that (51) and (52) become identical for $x=y=1/\sqrt{2}$ so that the doubling map gets the vector,

$$|W_3\rangle = \frac{1}{\sqrt{2}}|1\rangle \otimes |1\rangle + \frac{1}{2}(|2\rangle \otimes |2\rangle + |3\rangle \otimes |3\rangle), \tag{53}$$

which has fidelity

$$F = |\langle \Psi | W_3 \rangle|^2 = \frac{1}{2} + \sqrt{\frac{2}{3}} = p + (1-p) \frac{8}{9}, \quad 0 < p = 3\sqrt{6} - \frac{7}{2} < 1. \tag{54}$$

Let us now consider the state

$$\rho_F = p|\Psi\rangle\langle\Psi| + (1-p)|\Phi_{8/9}\rangle\langle\Phi_{8/9}|. \tag{55}$$

By using (48), it can be shown that its entanglement $E(\rho_F)$ is larger than $pE(\rho(1)) + (1-p)E(\rho(8/9))$ for $0 < p < 1$. This implies that convexity of $\mathcal{S}(F)$ in (32) is lost for $F > F^{**}$ in accordance with the discussion above.

We finally note that one can extend (49) to all dimensions larger than two. Indeed, let z_1, z_2 denote the components of a unit vector in two dimensions. By similar arguments one proves that the leaves of case 1 of the previous section are mapped onto certain leaves belonging to the entanglement of formation in $d+1$ dimensions by the embeddings

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \rightarrow z_1|00\rangle + (z_2/\sqrt{d}) \sum_{j=2}^{d+1} |jj\rangle. \quad (56)$$

In particular, the embeddings of $\{z_1, z_2\}$ and $\{z_2^*, z_1^*\}$ form an optimal pair with respect to the entanglement of formation. One further observes in the special case $z_1 = 1/\sqrt{d+1}$ the embeddings (56) are the totally symmetric vector Ψ in $d+1$ dimensions and

$$\sqrt{\frac{d}{d+1}}|11\rangle + \sqrt{\frac{1}{d(d+1)}} \sum_{j=2}^{d+1} |jj\rangle. \quad (57)$$

Its fidelity reads $F = 4d/(1+d)^2$, and we see as above

$$F_{d+1}^{**} = 4d(d+1)^{-2}, \quad (58)$$

i.e., the bifurcation value given in Ref. 11 for $d+1 > 2$.

IV. CONCLUSIONS

We have studied in several examples the entanglement defined by a maximal commuting subalgebra of a full matrix algebra, and its relation to the entanglement of formation. Apart from its actual numerical value, what is interesting is the structure of both entanglement functionals upon the space of states, and their separation into different leaves. To some extent these leaves can be found by applying group theoretical considerations. They show a rich structure with varying stability under the groups under consideration. Since the same group appears in different algebraic contexts, it can be shown that the decompositions of states on different algebras can be related. This helps to control the optimal decompositions and to understand their variety. This new technique is shown at work in several examples: The doubling map relates two quite different lines of research which had been considered almost independently up to now. In particular we have a further proof of the entanglement of formation results for isotropic states of Terhal and Vollbrecht in the region $(1/n) \leq F \leq F^{**}$.¹¹ Another embedding map verifies their bifurcation point F^{**} close to $F=1$ as a footprint of a symmetry-breaking in two dimensions. It belongs to a class of maps which change entanglement but not the leaves. The leaves are respected because the entanglements differ just by a convexly linear function.

We have provided some examples of embedding procedures which allow to connect various entanglement problems not only with each other, but also with problems involving other quantities based on convex or concave roofs, for example general entanglement monotones or Holevo (1-shot) capacities.

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