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Maximally entangled mixed symmetric states of two qubits

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In this work, a variation of the problem originally solved by Verstraete, Audenaert, and De Moor [Phys. Rev. A **64**, 012316 (2001)] on what is the maximum entanglement that can be created in a two-qubit system by a global unitary transformation is considered and solved when permutation invariance in the state is imposed. The additional constraint of permutation symmetry appears naturally in the context of bosonic systems or spin states. We also characterise symmetric two-qubit states that remain separable after any global unitary transformation, called symmetric absolutely separable states (SAS), or absolutely classical for spin states. This allows us to determine the maximal radius of a ball of SAS states around the maximally mixed state in the symmetric sector, and the minimal radius of a ball that includes the set of SAS states. For three-qubit systems, a necessary condition for absolute separability of symmetric states is given, which leads us to upper bounds on the ball radii similar to those studied for the two-qubit system.

I. INTRODUCTION AND PROBLEM STATEMENT

Entanglement is both a fundamental concept of quantum theory and a central resource of quantum technology applications, ranging from quantum communication and cryptography, quantum sensing and metrology, quantum simulation to quantum computing [1–6]. In a multipartite quantum system, entanglement can be created by applying an appropriate unitary transformation on a pure product state. This transformation cannot be *local*, as local unitary operations cannot change the entanglement content of a state. *Global* unitary transformations, on the other hand, have the potential to increase the entanglement among the parties [7, 8]. They can be implemented from the unitary time evolution under a Hamiltonian describing e.g. interactions among the subsystems or between the subsystems and external driving fields or a tailored experimental device [9, 10]. As quantum mechanics is time reversible, this entanglement can also be removed by applying the inverse unitary transformation.

Although it is at the heart of many protocols leading to a quantum advantage, entanglement remains one of the most delicate quantum properties to preserve from unwanted interactions with the environment. When a system interacts with its surrounding, its state must be described by a density operator $\rho \in \mathcal{B}(\mathcal{H})$, where $\mathcal{B}(\mathcal{H})$ is the set of the bounded linear operators acting on the Hilbert space of the quantum states $\mathcal{H}$. System-environment interactions generally tend to deteriorate the coherence and decrease the entanglement content of a state. After a sufficiently long decoherence time, an initially entangled state may lose all its entanglement and become a mixed separable state ρ_{sep}. This can even reach a point where no *global* unitary transformation applied on ρ_{sep} is capable of creating entanglement. The state is then said to be Absolutely Separable (AS) [11]. For a given system, it is obviously of interest to know which states are absolutely separable, as these states are of little or no use for applications that require entanglement. More generally, it is important to know what is the maximum amount of entanglement that can be obtained from a mixed state by the sole application of unitary transformations. To answer this question, it is first necessary to choose a measure of entanglement [6], i.e., a scalar function $E(\rho)$ of quantum states that satisfies a series of conditions [6] such as $E(\rho) = 0$ if and only if ρ is separable. In this work, we will only deal with quantum states which can be represented by a two-qubit or a qubit-qutrit system – cases for which the Positive Partial Transpose (PPT) criterion is a necessary and sufficient condition for entanglement [12] – and use as a measure of entanglement the negativity, defined by

$$\mathcal{N}(\rho) \equiv 2 \max \left(0\,, -\Lambda_{\min}\right), \tag{1}$$

where $\Lambda_{\min}$ is the minimal eigenvalue of the partial transpose of ρ with respect to a subsystem A consisting of one or two qubits, ρ^{T_A}. Equipped with this entanglement measure, the aim is then to find, for any fixed state ρ, the optimal negativity $\max_U \mathcal{N}(U\rho U^\dagger)$ where the optimisation is performed over all possible unitary operations U on $\mathcal{H}$.

The emblematic case of a bipartite quantum system composed of two qubits, with Hilbert space $\mathcal{H} \simeq \mathbb{C}^2 \otimes \mathbb{C}^2 \simeq \mathbb{C}^4$, was solved in a seminal paper by Verstraete, Audenaert, and De Moor [13]. The goal in this case is to find which global unitary operation $U \in SU(4)$ maximizes the entanglement of $U\rho U^\dagger$, i.e. which state in the $SU(4)$-orbit of ρ is maximally entangled. The authors of [13] showed that for a state ρ with eigenvalues sorted

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in nonascending order $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \lambda_4$, the largest negativity that can be reached is given by

$$\max_{U\in SU(4)} \mathcal{N}(U\rho U^\dagger) = \max\left(0, \sqrt{(\lambda_1-\lambda_3)^2+(\lambda_2-\lambda_4)^2}-\lambda_2-\lambda_4\right). \tag{2}$$

A direct consequence of this result is that a state ρ is AS if and only if its spectrum is such that the right-hand side of Eq. (2) is zero, which occurs when

$$(\lambda_1-\lambda_3)^2 - 4\,\lambda_2\lambda_4 \leqslant 0\,. \tag{3}$$

In particular, a two-qubit state ρ cannot be AS if it has more than one zero eigenvalues, as then Eq. (3) cannot be fulfilled. For exactly one zero eigenvalue ($\lambda_4 = 0$), the state is AS if $(\lambda_1-\lambda_3)^2 \leqslant 0$, which is only possible when $\lambda_1 = \lambda_2 = \lambda_3 = 1/3$.

Other aspects concerning the set of AS states for bipartite systems have been discussed in the literature. To mention a few, it has been shown in [14] that AS states form a convex and compact set, and that one can construct operators to witness absolute separability. Recently, quantum maps that output absolutely separable states have been analysed in Ref. [8]. Similar questions about absolute versions of quantum properties over (global) unitary orbits have also been studied, such as for locality [15], unsteerability [16], non-negative conditional entropy [17], or quantum discord, see Ref. [18] for an overview.

In some cases, physical constraints impose a restriction on the set of unitary transformations that can be applied to a state [19, 20]. For instance, in systems of identical and indistinguishable bosons, such as photons, an N-qubit state has to be invariant under permutations. The set of physical states is thus reduced to the symmetric subspace $\vee^N\mathbb{C}^2 \equiv (\mathbb{C}^2)^{\vee N} \subset \otimes^N\mathbb{C}^2 \equiv (\mathbb{C}^2)^{\otimes N}$ of dimension $N+1$, and hence the global unitary transformations are limited to $SU(N+1)$ operations. The questions posed above also arise naturally in this context, such as what is the maximum amount of entanglement in the $SU(N+1)$-orbit of a symmetric mixed state. Even for the simplest case of two qubits, this question has not been answered. The main objective of this paper is to fill this gap. Our results allow us to characterize the set of separable symmetric two-qubit states that remain separable after arbitrary $SU(3)$ transformations in the symmetric sector, which we call symmetric absolutely separable (SAS) states. The same characterization of the SAS two-qubit states is obtained in [21] using a different technique. The questions mentioned above can be studied for the three-qubit system by applying the sufficient and necessary PPT criterion of the qubit-qutrit system.

In the language of spin states, the SAS states are the equivalents of the Absolutely Classical (AC) spin states introduced in Ref. [22], see Sec. II for more details on the correspondence. Following notations similar to those of Ref. [8], we will denote by $\mathcal{A}_{\rm sym}$ the set of SAS states. As symmetric two-qubit states are of rank 3 at most (they have no component on the antisymmetric state), they cannot be AS with respect to their full $SU(4)$-orbit, except for the maximally mixed state in the symmetric subspace which we have shown previously is AS (as a special case of a state with eigenvalues $\lambda_1 = \lambda_2 = \lambda_3 = 1/3$). In contrast, we will see that the picture is much richer with the additional constraint of permutation symmetry, leaving room for a continuous two-dimensional set of SAS states. Indeed, balls full of SAS states exist around the maximally mixed state in the symmetric subspace [22]. These balls can be considered as the analogue of the balls of AS states around the maximally mixed state in the full Hilbert space, see e.g. Refs. [11, 23].

The present work is organised as follows: Sec. II reviews the definition of separability, classicality of spin states, and their absolute versions over global unitary operations. In Sec. III, we obtain the unitary transformation that maximizes the entanglement of any two-qubit symmetric mixed state, and present partial results for the case of three qubits. We then determine in Sec. IV the maximal radius of balls contained in $\mathcal{A}_{\rm sym}$ and the minimal ball that includes $\mathcal{A}_{\rm sym}$, both around the maximally mixed state in the symmetric sector, before concluding with Sec. V.

II. SEPARABILITY AND CLASSICALITY

A. Separable states of multiqubit systems

The Hilbert space $\mathcal{H}_1$ of a single qubit system is spanned by two basis vectors $|+\rangle$ and $|-\rangle$. The full Hilbert space of an N-qubit system $\otimes^N\mathcal{H}_1 \equiv \mathcal{H}_1^{\otimes N}$ is of dimension 2^N and is spanned by the product states $|\psi_1\rangle \otimes \cdots \otimes |\psi_N\rangle$ with $|\psi_k\rangle \in \{|+\rangle, |-\rangle\}$ for all $k = 1,\ldots,N$. The convex hull of the product states defines the set of *separable* states $\mathcal{S} \subset \mathcal{B}(\mathcal{H}_1^{\otimes N})$. Any state ρ that is not separable, i.e. $\rho \notin \mathcal{S}$, is said to be entangled. All separable states $\rho_{\rm sep} \in \mathcal{S}$ have zero negativity, $\mathcal{N}(\rho_{\rm sep}) = 0$. For $N = 2$ qubits, we also have that ρ is entangled only when $\mathcal{N}(\rho) \neq 0$. The measure of entanglement of a state cannot, by definition, be modified by local unitary operations [6]. On the other hand, the entanglement of a state ρ may change under a global unitary operation $U \in SU(2^N)$. However, there are special states that remain separable for all $U \in SU(2^N)$ and these are called *absolutely separable* (AS) states [11]. They can be defined as the states $\rho \in \mathcal{B}(\mathcal{H}_1^{\otimes N})$ for which

$$\max_{U\in SU(2^N)} E(U\rho U^\dagger) = 0 \tag{4}$$

for some measure of entanglement E.

B. Separable states in the symmetric sector and classical spin states

A multiqubit system is equivalent to a system of N spin-1/2, where each of the spin Hilbert spaces are spanned by the eigenvectors of the angular momentum operator S_3, the $|1/2, \pm 1/2\rangle$ states that we can identify with the $|\pm\rangle$ qubit states.

The symmetric sector $\vee^N \mathcal{H}_1 \equiv \mathcal{H}_1^{\vee N}$ of $\mathcal{H}_1^{\otimes N}$ is spanned by the symmetric Dicke states $|D_N^{(k)}\rangle$ for $k = 0, \dots N$, defined as [24]

$$|D_N^{(k)}\rangle = K \sum_{\pi} \pi\big(\underbrace{|+\rangle \otimes \dots |+\rangle}_{N-k} \otimes \underbrace{|-\rangle \otimes \dots |-\rangle}_{k} \big) , \quad (5)$$

where the sum runs over all the permutations π of the qubits and $K > 0$ is a normalization constant. In the spin picture, the $|D_N^{(k)}\rangle$ states are equivalent to the eigenvectors $|s, m\rangle$ of the collective S_3 operator, with $s = N/2$ and $m = (N-2k)/2$ [24]. Consequently, $\mathcal{H}_1^{\vee N}$ is isomorphic to the Hilbert space $\mathcal{H}^{(s)}$ of a spin s system, both being of dimension $N+1 = 2s+1$. Global unitary transformations restricted in $\mathcal{H}_1^{\vee N}$ correspond to $SU(N+1)$ transformations in $\mathcal{H}^{(s)}$.

The restriction of product states to the symmetric subspace leads to N-qubit states of the form $|\psi\rangle = |\phi\rangle^{\otimes N}$ with $|\phi\rangle = \alpha|+\rangle + \beta|-\rangle$ a normalized single qubit state. In the spin picture, this corresponds to *spin-coherent* (SC) states [25, 26]. The convex hull of SC states defines the set of *classical* spin-states $\mathcal{C}$ [27, 28]. A spin-s state $\rho^{(s)}$ is called *absolutely classical* (AC) when the $SU(2s+1)$-orbit of $\rho^{(s)} \in \mathcal{B}(\mathcal{H}^{(s)})$ is contained in $\mathcal{C}$ [22]. The complement of the set of classical states has also been studied in the literature [27–31] and a measure of non-classicality called quantumness has been defined in [29] as the distance between a state $\rho^{(s)}$ and $\mathcal{C}$ [30].

Here, we introduce the notion of *symmetric absolutely separable* (SAS) states (called absolutely symmetric separable states in Ref. [21]), the set of which will be denoted by $\mathcal{A}_{\text{sym}}$. A symmetric state $\rho_S \in \mathcal{B}(\mathcal{H}_1^{\vee N})$ will be called SAS if its $SU(N+1)$-orbit

$$\{U_S \rho_S U_S^\dagger : U_S \in SU(N+1)\} \quad (6)$$

contains only separable symmetric states. Equivalently, ρ_S is SAS if

$$\max_{U_S \in SU(N+1)} E(U_S \rho_S U_S^\dagger) = 0 \quad (7)$$

for some measure of entanglement E. The equivalence between the set of SAS states and the set of AC states (as proved by Theorem 1 of [32]) means that they can both be labeled by $\mathcal{A}_{\text{sym}}$, and both sets will satisfy the results deduced in the subsequent sections. From now on, we only use the terminology of SAS states in the symmetric sector $\mathcal{H}_1^{\vee N}$ for simplicity.

C. SAS states for $2 \times m$ bipartite systems

To highlight the difference between SAS and AS states, we can use a general result of Johnston [33] which says that a $2 \times m$ bipartite state ρ with spectrum $\lambda_1 \geqslant \lambda_2 \geqslant \dots \geqslant \lambda_{2m} \geqslant 0$ is AS if and only if

$$\lambda_1 \leqslant \lambda_{2m-1} + 2\sqrt{\lambda_{2m-2}\lambda_{2m}}. \quad (8)$$

An implication of this result is that no symmetric state of N qubits can be AS for $N > 2$. Indeed, let ρ be an N-qubit state viewed as a $2 \times 2^{N-1}$ bipartite state. Then ρ is AS if and only if $\lambda_1 \leqslant \lambda_{2^N-1} + 2\sqrt{\lambda_{2^N-2}\lambda_{2^N}}$. But for symmetric states, which have support only on the symmetric subspace, $\lambda_k = 0 \ \forall\ k \geqslant N+1$, which leads to the condition $\lambda_1 \leqslant 0$ that can never be fulfilled since $\lambda_1 > 0$ is the largest eigenvalue of ρ. Although symmetric multiqubit states of more than two qubits cannot be AS, they can be SAS as we show below.

III. MAIN RESULTS

A. Two qubits

The central question presented in the introduction can now be reformulated as follows: For a symmetric two-qubit mixed state ρ_S, what is the maximum entanglement that can be obtained by a global unitary transformation $U_S \in SU(3)$ that leaves the symmetric sector invariant ?

The answer to this question and the main result of this paper is stated by the following theorem:

Theorem 1 *Let ρ_S be a symmetric two-qubit state with spectrum $\tau_1 \geqslant \tau_2 \geqslant \tau_3$. It holds that*

$$\begin{aligned} &\max_{U_S \in SU(3)} \mathcal{N}\left(U_S \rho_S U_S^\dagger\right) = \\ &\qquad \max\left(0, \sqrt{\tau_1^2 + (\tau_2 - \tau_3)^2} - \tau_2 - \tau_3\right), \end{aligned} \quad (9)$$

where the maximal negativity is reached by the state $\tilde{\rho}_S = U_S \rho_S U_S^\dagger$ given up to local unitary transformations by

$$\tilde{\rho}_S = \tau_3 |D_2^{(0)}\rangle\langle D_2^{(0)}| + \tau_1 |D_2^{(1)}\rangle\langle D_2^{(1)}| + \tau_2 |D_2^{(2)}\rangle\langle D_2^{(2)}| . \quad (10)$$

The following Corollary then follows immediately from Theorem 1:

Corollary 1 *Let ρ_S be a symmetric two-qubit state with spectrum $\tau_1 \geqslant \tau_2 \geqslant \tau_3$. Then $\rho_S \in \mathcal{A}_{\text{sym}}$ if and only if its eigenvalue spectrum fulfills*

$$\sqrt{\tau_2} + \sqrt{\tau_3} \geqslant 1 . \quad (11)$$

Proof. The symmetric two-qubit state ρ_S is SAS if the right-hand side of (9) is zero which, using the normalization condition $\tau_1 + \tau_2 + \tau_3 = 1$, is equivalent to

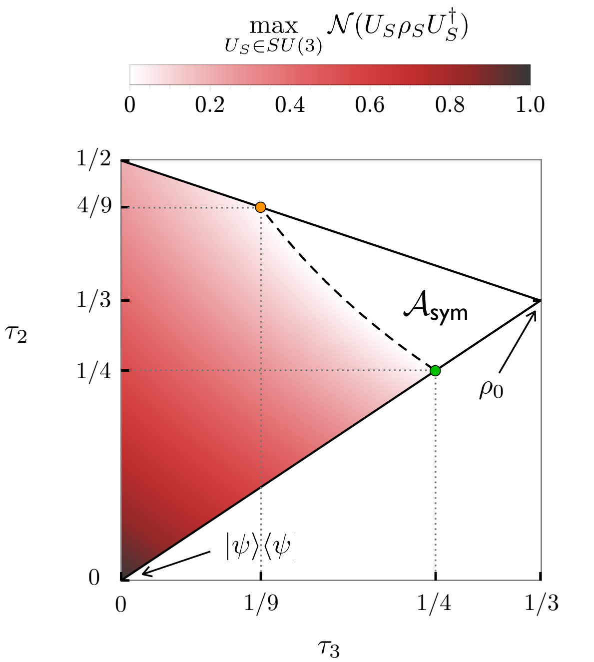

FIG. 1. Density plot of the maximum negativity (9) attained in the $SU(3)$-orbit of a symmetric two-qubit state ρ_S over the simplex of its eigenvalues (τ_3, τ_2). The dashed curve shows the boundary of the set $\mathcal{A}_{\rm sym}$ of SAS states given by Corollary 1, with end points being represented by orange and green dots respectively. The right corner of the simplex corresponds to the maximally mixed symmetric state, $\rho_0 = \mathbb{1}_3/3 \in \mathcal{B}(\mathcal{H}_1^{\vee 2})$, and the lower corner to a pure state.

the above inequality. □

In Fig. 1, we show a density plot of the maximal negativity given by Eq. (9) for all states $\rho_S \in \mathcal{B}(\mathcal{H}_1^{\vee 2})$ in terms of its two smallest eigenvalues τ_2 and τ_3. The 2-dimensional white region constitutes the set $\mathcal{A}_{\rm sym}$ and its bounds are given by two inequalities associated with the eigenvalues sorting, $\tau_2 \geqslant \tau_3$ and $2\,\tau_2 + \tau_3 \leqslant 1$ (solid lines), and Eq. (11) (dashed line). In particular, the solid lines correspond to the states with two coincident spectrum eigenvalues, $\tau_2 = \tau_3$ or $\tau_1 = \tau_2$, respectively. The end points of the bound defined by Eq. (11) correspond to the states with spectrum $(\tau_1, \tau_2, \tau_3) = (4/9, 4/9, 1/9)$ (orange dot) and $(1/2, 1/4, 1/4)$ (green dot). Lastly, let us also remark that when $\rho_S \in \mathcal{B}(\mathcal{H}_1^{\vee 2})$ has one zero eigenvalue $\tau_3 = 0$, the condition (11) cannot be met and then $\rho_S \notin \mathcal{A}_{\rm sym}$, as can be seen in Fig. 1.

Numerics shows that the maximal concurrence in the $SU(3)$-orbit of a symmetric two-qubit state is also reached for the state (10). A direct calculation shows that the concurrence of (10) is

$$C(\tilde{\rho}_S) = \max\left(0, \tau_1 - 2\sqrt{\tau_2 \tau_3}\right). \tag{12}$$

We end this subsection with the proof of Theorem 1, which follows a reasoning similar to that of Ref. [13].

Proof of Theorem 1. The minimal eigenvalue $\Lambda_{\min}$ of the partial transpose of ρ_S with respect to one qubit, $\rho_S^{T_A}$, is equivalent to [13, 21]

$$\Lambda_{\min} = \min_{|\psi\rangle \in \mathcal{H}_1^{\otimes 2}} \mathrm{Tr}\left[\rho_S (|\psi\rangle\langle\psi|)^{T_A}\right] . \tag{13}$$

The general two-qubit state $|\psi\rangle$ can be written as a linear superposition of a symmetric state and an antisymmetric state, $|\psi_S\rangle \in \mathcal{H}_1^{\vee 2}$ and $|\psi_A\rangle \in \mathcal{H}_1^{\wedge 2}$,

$$|\psi\rangle = \cos\alpha\, |\psi_S\rangle + e^{i\delta} \sin\alpha\, |\psi_A\rangle , \tag{14}$$

where $\alpha \in [0, \pi/2]$ and $\delta \in [0, 2\pi)$. On the one hand, $|\psi_S\rangle$ can be written via the Schmidt decomposition as

$$|\psi_S\rangle = \cos\beta\, |n_1\rangle \otimes |n_1\rangle + \sin\beta\, |n_2\rangle \otimes |n_2\rangle , \tag{15}$$

where $\Gamma = \{|n_j\rangle\}_{j=1}^2$ is an orthogonal basis of $\mathcal{H}_1$ and $\beta \in [0, \pi/2]$ [34]. On the other hand, $|\psi_A\rangle$ can be written for any orthogonal basis of $\mathcal{H}_1$, in particular Γ, as

$$|\psi_A\rangle = \frac{1}{\sqrt{2}} \left(|n_1\rangle \otimes |n_2\rangle - |n_2\rangle \otimes |n_1\rangle\right) . \tag{16}$$

Hence, $|\psi\rangle\langle\psi|$ is the sum of four terms

$$\begin{aligned} |\psi\rangle\langle\psi| =& \cos^2\alpha\, |\psi_S\rangle\langle\psi_S| + \sin^2\alpha\, |\psi_A\rangle\langle\psi_A| \\ &+ \cos\alpha \sin\alpha\, \left(e^{-i\delta} |\psi_S\rangle\langle\psi_A| + e^{i\delta}\, |\psi_A\rangle\langle\psi_S|\right) . \end{aligned} \tag{17}$$

The condition for a state ρ_S to be symmetric is that it has support only on the symmetric sector of $\mathcal{B}(\mathcal{H}_1^{\otimes 2})$, which can be written as $\rho_S = P_S \rho_S P_S$ with P_S the projection operator onto $\mathcal{H}_1^{\vee 2}$. For convenience, we now introduce the symmetrized state $|n_1, n_2\rangle$ resulting from the action of P_S on the product state $|n_1\rangle \otimes |n_2\rangle$,

$$P_S |n_1\rangle \otimes |n_2\rangle = \frac{1}{2} \left(|n_1\rangle \otimes |n_2\rangle + |n_2\rangle \otimes |n_1\rangle\right) \equiv \frac{|n_1, n_2\rangle}{\sqrt{2}}.$$

Replacing ρ_S in Eq. (13) by $P_S \rho_S P_S$ and using the cyclic property of the trace, we get

$$\Lambda_{\min} = \min_{|\psi\rangle \in \mathcal{H}_1^{\otimes 2}} \mathrm{Tr}\left[\rho_S P_S (|\psi\rangle\langle\psi|)^{T_A} P_S\right] = \min_X \mathrm{Tr}\left[\rho_S X\right] ,$$

where the operator $X = P_S (|\psi\rangle\langle\psi|)^{T_A} P_S$ can be developed as

$$X = \cos^2\alpha\, \Sigma_1 + \sin^2\alpha\, \Sigma_2 + \cos\alpha \sin\alpha \sin\delta\, \Sigma_3 \tag{18}$$

where the Σ_j operators are represented in the orthonormal basis $\Gamma' = \{|n_1\rangle^{\otimes 2}, |n_1, n_2\rangle, |n_2\rangle^{\otimes 2}\}$ by the matrices

$$\Sigma_1 = \begin{pmatrix} \cos^2\beta & 0 & 0 \\ 0 & \cos\beta \sin\beta & 0 \\ 0 & 0 & \sin^2\beta \end{pmatrix} , \tag{19}$$

$$\Sigma_2 = \frac{1}{2} \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} , \tag{20}$$

$$\Sigma_3 = i \begin{pmatrix} 0 & \cos\beta & 0 \\ -\cos\beta & 0 & \sin\beta \\ 0 & -\sin\beta & 0 \end{pmatrix} . \tag{21}$$

The basis Γ' can be transformed to the symmetric Dicke basis $\{|D_2^{(k)}\rangle\}_{k=0}^2$ by a diagonal $SU(2)\times SU(2)$-transformation $V=\tilde{V}\otimes\tilde{V}$ such that $\tilde{V}^\dagger|n_1\rangle=|+\rangle$ and $\tilde{V}^\dagger|n_2\rangle=|-\rangle$. Hence, $P_S(|\psi\rangle\langle\psi|)^{T_A}P_S$ for a general state $|\psi\rangle$ is parametrized by the (α,β,δ) variables and a diagonal $SU(2)\times SU(2)$-transformation V

$$P_S(|\psi\rangle\langle\psi|)^{T_A}P_S=V^\dagger XV\,, \tag{22}$$

where the matrix X written in the symmetric Dicke basis has the form (18). The smallest value of $\Lambda_{\min}$ over the $SU(3)$-orbit of ρ_S is equal to

$$\min_{U\in SU(3)}\Lambda_{\min}=\min_{U,V,\alpha,\beta,\delta}\mathrm{Tr}\left[U\rho_S U^\dagger V^\dagger XV\right]\,. \tag{23}$$

Without loss of generality, the U and V unitary transformations can be combined to $W=VU$ because the diagonal $SU(2)\times SU(2)$ transformation V is in the $SU(3)$ group [35]. The minimization problem then reduces to

$$\min_{\substack{W\in SU(3)\\ \alpha,\beta,\gamma}}\mathrm{Tr}\left[\rho_S W^\dagger XW\right]\,. \tag{24}$$

The Birkhoff's theorem (Theorem 8.7.2 of [36]) establishes that the minimum over all $W\in SU(3)$ is attained when W is the product of matrices diagonalizing ρ_S and X in the same basis, and a matrix $W(\pi)$ representing a permutation $\pi\in S_3$ where S_3 is the permutation group of three elements. Without loss of generality, we consider ρ_S and X to be represented by the diagonal matrices ρ_d and X_d in the Dicke basis. Thus, (24) is given by

$$\min_{\substack{\pi\in S_3\\ \alpha,\beta,\gamma}}\mathrm{Tr}\left[\rho_d W^\dagger(\pi)X_dW(\pi)\right]=\min_{\substack{\pi\in S_3\\ \alpha,\beta,\gamma}}\sum_{k=1}^3\tau_{\pi(k)}\xi_k\,,$$

where ξ_k are the eigenvalues of X. The eigenvalues ξ_k cannot generally be expressed in a compact way. However, the function to minimize in the last equation must have its derivative with respect to δ equal to zero at W,α,β,δ where the minimum is attained, which implies that

$$\mathrm{Tr}\left[\rho_S W^\dagger\Sigma_3 W\right]\cos\alpha\sin\alpha\cos\delta=0. \tag{25}$$

The latter equation is satisfied either by one of the following solutions: (A) $\delta=\pi/2\,,3\pi/2$, or (B) $\alpha=0\,,\pi/2$, or (C) when $\mathrm{Tr}[\rho_S W^\dagger\Sigma_3 W]=0$. First, the eigenvalues for the solution (A) are the same for both values of δ and equal to

$$\begin{pmatrix}\xi_1\\ \xi_2\\ \xi_3\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1+\sqrt{1-z^2}\\ z\\ 1-\sqrt{1-z^2}\end{pmatrix}\,, \tag{26}$$

with $z=-\sin^2\alpha+\cos^2\alpha\sin(2\beta)$. On the other hand, while the solution (B) keeps only Σ_1 or Σ_2 in X [see Eq. (18)], the solution (C) restricts the available set of the W matrices to $\mathcal{R}_\beta=\{W\in SU(3)|\mathrm{Tr}\left[\rho_S W^\dagger\Sigma_3 W\right]=0\}$ with $\Sigma_3=\Sigma_3(\beta)$. Then, Eq. (24) for the solution (C) is reduced and lower bounded by

$$\begin{aligned}&\min_{\substack{W'\in\mathcal{R}_\beta\\ \alpha,\beta,\gamma}}\mathrm{Tr}\left[\rho_S W'^\dagger XW'\right]\\ &=\min_{\substack{W'\in\mathcal{R}_\beta\\ \alpha,\beta,\gamma}}\mathrm{Tr}\left[\rho_S W'^\dagger(\cos^2\alpha\Sigma_1+\sin^2\alpha\Sigma_2)W'\right]\\ &\geqslant\min_{\substack{W\in SU(3)\\ \alpha,\beta,\gamma}}\mathrm{Tr}\left[\rho_S W^\dagger(\cos^2\alpha\Sigma_1+\sin^2\alpha\Sigma_2)W\right]\,. \end{aligned} \tag{27}$$

Thus, the solution (B) and the upper bound of (C) can be studied simultaneously by omitting Σ_3 in the minimization problem, leaving $X=\cos^2\alpha\Sigma_1+\sin^2\alpha\Sigma_2$ with eigenvalues equal to

$$\begin{pmatrix}\xi_1\\ \xi_2\\ \xi_3\end{pmatrix}=\frac{1}{4}\begin{pmatrix}1+y_1-\sqrt{2(1+y_1^2-2y_2^2)}\\ 1+y_1+\sqrt{2(1+y_1^2-2y_2^2)}\\ 1-y_1+2y_2\end{pmatrix} \tag{28}$$

where $y_1=\cos(2\alpha)$ and $y_2=\cos^2\alpha\sin(2\beta)$. For both sets of eigenvalues (26) and (28), we must now find the critical points of (25) with respect to the variables α and β. We enlist in Appendix A all the critical points obtained for the cases mentioned above. By comparing the values obtained for (25) with all the possible permutations π, we deduce that the minimum $\Lambda_{\min}$ in the $SU(3)$-orbit of ρ_S is reached for the solution (A) with

$$z=-\sin^2\alpha+\cos^2\alpha\sin(2\beta)=-\frac{\tau_1}{\sqrt{\tau_1^2+(\tau_2-\tau_3)^2}} \tag{29}$$

and with π such that

$$\begin{aligned}\Lambda_{\min}&=\tau_3\,\xi_1+\tau_1\,\xi_2+\tau_2\,\xi_3\\ &=\frac{1}{2}\left(\tau_2+\tau_3-\sqrt{\tau_1^2+(\tau_2-\tau_3)^2}\right).\end{aligned} \tag{30}$$

It is this value of $\Lambda_{\min}$ which gives the expression (9) for the negativity $\mathcal{N}(\rho_S)$. In particular, for $\alpha=0$ and $\sin(2\beta)=-\tau_1/\sqrt{\tau_1^2+(\tau_2-\tau_3)^2}$, the X matrix is already diagonal in the symmetric Dicke basis and reads

$$X=\xi_1|D_2^{(0)}\rangle\langle D_2^{(0)}|+\xi_2|D_2^{(1)}\rangle\langle D_2^{(1)}|+\xi_3|D_2^{(2)}\rangle\langle D_2^{(2)}|.$$

In order to attain (30), ρ_S must then be equal to (10), up to a local unitary transformation. □

Let us remark that the minimization in (13) is performed over all states $|\psi\rangle\in\mathcal{H}_1^{\otimes 2}$, and we found that the states $|\psi\rangle$ that minimize $\Lambda_{\min}$ over the $SU(3)$-orbit of ρ are of the form (14), with $\delta=\pi/2,\,3\pi/2$ and (α,β) such that Eq. (29) is satisfied. This implies that there exists a 1-dimensional set of states $|\psi\rangle\in\mathcal{H}_1^{\otimes 2}$ that minimize $\Lambda_{\min}$ of ρ_S. In particular, for $\alpha=0$, the state $|\psi\rangle$ belongs to the symmetric sector $\mathcal{H}_1^{\vee 2}$. The problem of finding the minimal eigenvalue of $\rho_S^{T_A}$ when the state $|\psi\rangle$

is restricted in the symmetric sector $|\psi\rangle \in \mathcal{H}_1^{\vee 2}$ was studied recently in [21], where they also reported the same characterization of SAS states as given in our Corollary 1.

B. Three qubits

In the case of symmetric three-qubit states $\rho_S \in \mathcal{B}(\mathcal{H}_1^{\vee 3})$, the determination of the maximally entangled state in the $SU(4)$-orbit of an arbitrary state ρ_S can again be formulated as an optimization problem with the negativity as objective function because the PPT criterion is both a necessary and sufficient condition for entanglement in the qubit-qutrit system [12], for which $\mathcal{H}_1^{\vee 3}$ is a subspace. However, optimisation seems to be much more difficult in this case and remains an open problem at this stage. Nevertheless, it is possible to obtain necessary conditions for the absolute separability of a state (with respect to $SU(4)$ transformations and not global unitaries in the full Hilbert space). We start with the following observation.

Observation 1 *A symmetric three-qubit state ρ_S cannot be SAS if its spectrum $\tau_1 \geqslant \tau_2 \geqslant \tau_3 \geqslant \tau_4$ satisfies*

$$\tau_2 < 1 - \tau_3 - \tau_4 - \sqrt{3\,\tau_3\tau_4} \quad \wedge \quad \tau_3 > 0\,. \tag{31}$$

Proof. First, any symmetric state ρ_S with spectrum $\tau_1 \geqslant \tau_2 \geqslant \tau_3 \geqslant \tau_4$ can be brought by a unitary transformation to the state

$$\begin{aligned}\rho_S' = {} & \tau_4\,|D_3^{(3)}\rangle\langle D_3^{(3)}| \,+\, \tau_1\,|D_3^{(2)}\rangle\langle D_3^{(2)}| \\ & + \tau_3\,|D_3^{(1)}\rangle\langle D_3^{(1)}| \,+\, \tau_2\,|D_3^{(0)}\rangle\langle D_3^{(0)}|\,.\end{aligned} \tag{32}$$

The partial transpose of ρ_S' with respect to any of the bipartitions has as its lowest eigenvalue

$$\lambda_{\min} = \frac{1}{6}\left(3\,\tau_4 + 2\,\tau_3 - \sqrt{p(\tau_2,\tau_3,\tau_4)}\right)\,, \tag{33}$$

with

$$\begin{aligned}p(\tau_2,\tau_3,\tau_4) = {} & 8 - 16\,\tau_4 + 17\,\tau_4^2 - 16\,\tau_3 \\ & + 4\,\tau_4\tau_3 + 12\,\tau_3^2 - 16\,\tau_2 \\ & + 16\,\tau_4\tau_2 + 16\,\tau_3\tau_2 + 8\,\tau_2^2\,.\end{aligned} \tag{34}$$

It is then easy to verify that the lowest eigenvalue (33) is negative, hence the state ρ_S' is entangled by the PPT criterion if and only if the condition (31) is met. In this case, ρ_S is not absolutely separable because it is unitarily equivalent to the entangled state ρ_S'. □

The condition (31) is the strictest condition that can be obtained by applying the PPT criterion to a mixture of symmetric Dicke states of the form (32) and considering all possible permutations of the eigenvalues as weights of the mixture. It places strong constraints on the spectrum of a state for it to be potentially AS. However, this is only a sufficient condition for a state not to be AS, as one can find states that do not satisfy (31) but are nevertheless not AS. We provide here an example of such state. Consider the state $\rho_S'' = U_S \rho_S' U_S^\dagger$ obtained by application of the unitary operator expressed in the basis $\{|D_3^{(k)}\rangle\}_{k=0}^3$ by the matrix

$$U_S = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \end{pmatrix} \tag{35}$$

on the state ρ_S' given by Eq. (32) with $\tau_1 = 0.362191$, $\tau_2 = 0.213809$, $\tau_3 = 0.213$ and $\tau_4 = 0.211$. The state ρ_S'' has a negative partial transpose but violates condition (31) because we have $\tau_2 - \left(1 - \tau_3 - \tau_4 - \sqrt{3\,\tau_3\tau_4}\right) \approx 0.005 > 0$.

IV. IMPROVED BOUNDS ON THE PURITY OF SAS STATES

In this section, we deduce from the previous results bounds of the radius of the maximal ball contained in $\mathcal{A}_{\rm sym}$ and the minimal ball that includes $\mathcal{A}_{\rm sym}$, both centred on the maximally mixed symmetric state $\rho_0 \propto \mathbb{1}$. These balls have been studied recently in [37, 38] in the full-Hilbert space for qubit-qudit systems. We first define the distance r between a state ρ_S and ρ_0 through the decomposition

$$\rho_S = \rho_0 + r\,\tilde{\rho}_S \tag{36}$$

where $\tilde{\rho}_S$ is such that $\mathrm{Tr}[\tilde{\rho}_S] = 0$ and $\mathrm{Tr}[\tilde{\rho}_S^2] = 1$ [27]. A simple calculation shows that, for a spin s, the distance r is related to the purity of ρ_S by

$$r = \sqrt{\mathrm{Tr}\left[\rho_S^2\right] - \frac{1}{2s+1}}\,. \tag{37}$$

The range for r is $\left[0, \sqrt{\frac{2s}{2s+1}}\,\right]$, where the upper and lower limits are reached when ρ_S is equal to ρ_0 or any pure state, respectively. As in the non-symmetric case, there are balls centred on ρ_0 containing only SAS states. In other words, there exists a maximum radius $r_{\rm SAS}$ such that any ball centred on ρ_0 with radius $r \leqslant r_{\rm SAS}$ contains only SAS states. A lower bound for $r_{\rm SAS}$ has been determined in Ref. [22] in the context of the absolute classicality of spin-s states (in correspondence with $2s$-qubit symmetric states). It is given by

$$r_{\rm SAS}^{\rm LB} = \frac{1}{\sqrt{(4s+2)\left[(4s+1)\binom{4s}{2s} - (s+1)\right]}}. \tag{38}$$

For two qubits, we can calculate the exact value of $r_{\rm SAS}$ using the results of the previous section. First, we calculate the radius r of the states (10) that maximize the negativity in each $SU(3)$-orbit and get, using the normalization condition $\tau_1 + \tau_2 + \tau_3 = 1$,

$$r^2 = \frac{2}{3} + 2\left(\tau_2^2 + \tau_3^2 + \tau_2\tau_3 - \tau_2 - \tau_3\right). \tag{39}$$

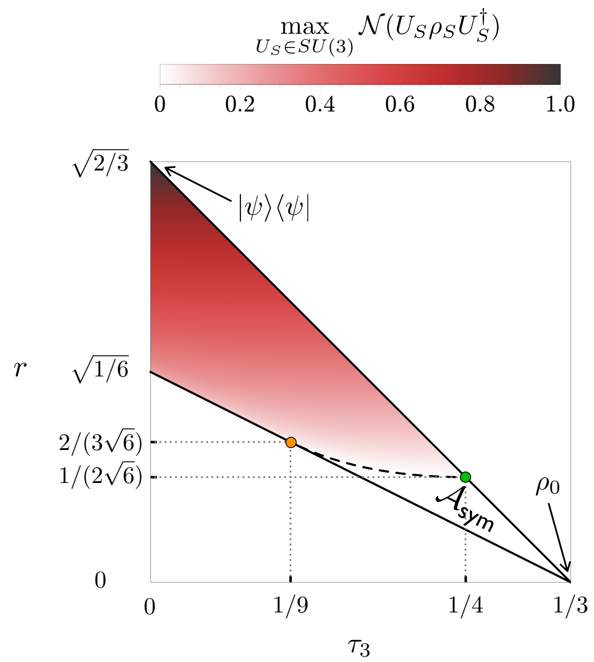

FIG. 2. Density plot of the maximal negativity (9) over the simplex of symmetric two-qubit states ρ_S parametrized with (τ_3, r). The dashed line shows the border with the set of SAS states [see Eq. (40)].

The last equation allows us to express τ_2 in terms of r and τ_3, and thus the maximum negativity over each $SU(3)$-orbit of ρ_S, Eq. (9), as a function of τ_3 and r. In Fig. 2, we show a density plot of this maximum negativity, where the variables τ_3 and r are subject to the constraints $\sqrt{2/3}\,(1-3\tau_3) \geqslant r \geqslant (1-3\tau_3)/\sqrt{6}$ depicted by straight lines. The set $\mathcal{A}_{\rm sym}$ (white region) delimited by the dashed curve corresponds to the inequality

$$r \leqslant \sqrt{\frac{2}{3}}\left[1+3\left(\tau_3-\sqrt{\tau_3}\right)\right], \quad \tau_3 \in \left[\frac{1}{9},\frac{1}{3}\right]. \tag{40}$$

The end points of the dashed curve, shown by the orange and green dots, have coordinates (τ_3, r) given by

$$\left(\frac{1}{9},\frac{2}{3\sqrt{6}}\right) \quad \text{and} \quad \left(\frac{1}{4},\frac{1}{2\sqrt{6}}\right) \tag{41}$$

respectively, and they correspond to the same states as those shown in Fig. 1. As a result, all states with $r \leqslant 1/(2\sqrt{6})$ are necessarily SAS, from which we deduce that $r_{\rm SAS} = 1/(2\sqrt{6})$. This value is strictly larger than that provided by Eq. (38), equal to $1/(2\sqrt{42})$ for $s = N/2 = 1$. Another interesting observation is that there exists a ball with minimal radius $R_{\rm SAS}$ that includes $\mathcal{A}_{\rm sym}$. From Fig. 1, it is easy to see that this radius is the r coordinate of the orange dot or $R_{\rm SAS} = 2/(3\sqrt{6})$. Therefore, any state ρ_S at a distance from ρ_0 larger than $R_{\rm SAS}$ cannot be SAS.

For $N=3$, the three-dimensional simplex associated with the spectrum eigenvalues (τ_2,τ_3,τ_4) of a symmetric

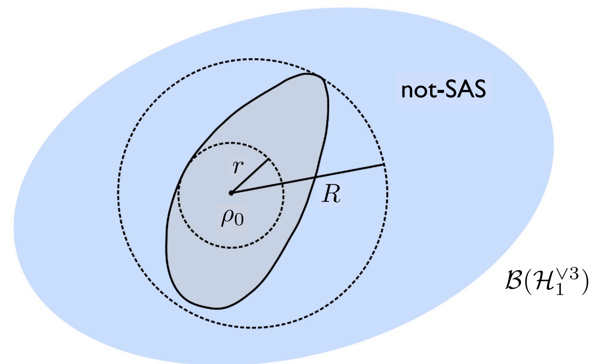

FIG. 3. Sketch of the set of states $\rho_S \in \mathcal{B}(\mathcal{H}_1^{\vee 3})$ which satisfy Obs. 1, represented by the outer (blue) region. While the outer region is composed only of non-SAS states, the set $\mathcal{A}_{\rm sym}$ is contained in the inner (gray) region. The balls of radii R and r define the upper bounds of $R_{\rm SAS}$ and $r_{\rm SAS}$, respectively.

three-qubit mixed state, sorted in non-ascending order $\tau_1 \geqslant \tau_2 \geqslant \tau_3 \geqslant \tau_4$ and with $\tau_1 = 1-\tau_2-\tau_3-\tau_4$, is divided into two regions by the conditions of Obs. 1, Eq. (31), as shown in Fig. 3. While the outer (blue) region consists only of not-SAS states, the inner (gray) region includes $\rho_0 = (1/4)\mathbb{1}_4$ and $\mathcal{A}_{\rm sym}$. Hence, the minimal (maximal) distance r from ρ_0 to the boundary between the regions gives an upper bound for $r_{\rm SAS}$ ($R_{\rm SAS}$). The distance r of a state that satisfies the equality of Eq. (31) can be written in terms of the (τ_3,τ_4) variables as

$$r^2 = \left(\tau_3-\frac{1}{4}\right)^2+\left(\tau_4-\frac{1}{4}\right)^2+\left(\sqrt{3\tau_3\tau_4}-\frac{1}{4}\right)^2 + \left(\tau_3+\tau_4+\sqrt{3\tau_3\tau_4}-\frac{3}{4}\right)^2, \tag{42}$$

and the minimal distance is given by

$$r = \frac{\sqrt{9-5\sqrt{3}}}{2\sqrt{6}}, \quad \text{for} \quad (\tau_3,\tau_4) = \left(\frac{3+\sqrt{3}}{24},\frac{3+\sqrt{3}}{24}\right).$$

Then, $r_{\rm SAS}$ has the following bounds

$$\frac{1}{10\sqrt{11}} \leqslant r_{\rm SAS} < \frac{\sqrt{9-5\sqrt{3}}}{2\sqrt{6}}, \tag{43}$$

where the lower bound comes from Eq. (38). On the other hand, the maximum distance R as given by Eq. (42) is obtained when $\tau_1=\tau_2=\tau_3$, or

$$R = \frac{\sqrt{3}}{10}, \quad \text{for} \quad (\tau_3,\tau_4) = \left(\frac{3}{10},\frac{1}{10}\right). \tag{44}$$

Therefore, since Obs. 1 is only a sufficient condition, $R_{\rm SAS} \leqslant \sqrt{3}/10$. Numerical calculations, however, seem to show that this is in fact a tight bound [39].

V. CONCLUSIONS

The problem we have studied and solved in this work is a variation of the original problem considered by Verstraete, Audenaert, and De Moor [13] on maximally entangled two-qubit states, when permutation symmetry is imposed. Our main result is the determination of the symmetric state with the maximal negativity in the $SU(3)$-orbit of any mixed symmetric state of two qubits (Theorem 1). As a direct application of our results, we have provided a full characterization of the SAS states based on their spectrum, and the maximal (minimal) radius of a ball contained in (containing) the SAS states. Bounds for the radii of the corresponding balls in the three-qubit system are also obtained, where we use a necessary condition deduced in Observation 1 for absolute separability of symmetric states under global unitary operations in the symmetric subspace. As the PPT entanglement criterion for three-qubit symmetric states is both necessary and sufficient, it should be possible to improve these results to achieve a complete characterization of the maximally entangled symmetric three-qubit state in each $SU(4)$-orbit. We also believe that a proof of the optimality of the state (10) for other measures of entanglement such as the concurrence (see Eq. (12) and the text above), which is supported by our numerical data, should be within reach with the same techniques used here.

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Appendix A: Critical points of Λ

Case 1: $\delta = \pi/2, 3\pi/2$. The X matrix has the same eigenvalues for both values of δ, given by Eq. (26). Setting $t_j = \tau_{\pi(j)}$, the critical points of (25) and its Λ-value are the following:

i) $t_2 \geqslant t_3$:

$$z = -\frac{t_1}{\sqrt{t_1^2 + (t_2 - t_3)^2}}, \quad \Lambda = \frac{1}{2}\left(t_2 + t_3 - \sqrt{t_1^2 + (t_2 - t_3)^2}\right). \tag{A1}$$

ii) $t_2 \leqslant t_3$:

$$z = \frac{t_1}{\sqrt{t_1^2 + (t_2 - t_3)^2}}, \quad \Lambda = \frac{1}{2}\left(t_2 + t_3 + \sqrt{t_1^2 + (t_2 - t_3)^2}\right). \tag{A2}$$

iii) $\alpha = \pi/2$, $\Lambda = (t_2 + t_3 - t_1)/2$.

iv) $\alpha = 0$ and $\beta = \pi/4$, $\Lambda = 1/2$.

Case 2: X without Σ_3. The eigenvalues of X are in this case given by (28). In addition to identical solutions to the previous case, other solutions appear which we list below:

i) $t_1 \geqslant t_2$:

$$y_1 = \frac{t_1 + t_2 - t_3}{\sqrt{1 - 8t_1t_2}}, \quad y_2 = -\frac{t_3}{\sqrt{1 - 8t_1t_2}}, \quad \Lambda = \frac{1}{4}\left(1 - \sqrt{1 - 8t_1t_2}\right). \tag{A3}$$

ii) $t_1 \leqslant t_2$:

$$y_1 = \frac{t_3 - t_1 - t_2}{\sqrt{1 - 8t_1t_2}}, \quad y_2 = \frac{t_3}{\sqrt{1 - 8t_1t_2}}, \quad \Lambda = \frac{1}{4}\left(1 + \sqrt{1 - 8t_1t_2}\right). \tag{A4}$$