
Entanglement and Quantumness - New Numerical Approaches -

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1. Abstract

1.1. English

The main topic of this compilation thesis is the investigation of multipartite entanglement of finite dimensional systems. We developed a numerical algorithm that detects if a multipartite state is entangled or separable in a finite number of steps of a semi-definite optimization task. This method is an extension of previously known semi-definite methods, which are inconclusive when the state is separable. In our case, if the state is separable, an explicit decomposition into a mixture of separable states can be extracted. This was achieved by mapping the entanglement problem onto the mathematically well studied truncated moment problem. Additionally, a new way of writing the partially transposed state for symmetric multi-qubit states was developed which simplifies many results previously known in entanglement theory. This new way of writing the partial transpose criterion unifies different interpretations and alternative formulations of the partial transpose criterion and it is also a part in the aforementioned semi-definite algorithm.

The geometric properties of entangled symmetric states of two qubits were studied in detail: We could answer the question of how far a given pure state is from the convex hull of symmetric separable states, as measured by the Hilbert-Schmidt distance, by giving an explicit formula for the closest separable symmetric state. For mixed states we could provide a numerical upper and analytical lower bound for this distance. For a larger number of qubits we investigated the ball of absolutely classical states, i.e. symmetric multi-qubit states that stay separable under any unitary transformation. We found an analytical lower bound for the radius of this ball around the maximally mixed symmetric state and gave a numerical upper bound on this radius, by searching for an entangled state as close as possible to the maximally mixed symmetric state.

The tensor representation of a symmetric multi-qubit state, or spin- j state, allowed us to study entanglement properties based on the spectrum of the tensor via tensor eigenvalues. The definiteness of this tensor relates to the entanglement of the state it represents

and, hence, the smallest tensor eigenvalue can be used to detect entanglement. However, the tensor eigenvalues are more difficult to determine than the familiar matrix eigenvalues which made the investigation computationally more challenging. The relationship between the value of the smallest tensor eigenvalue and the amount of entanglement in the state was also investigated. It turned out that they are strongly correlated for small system sizes, i.e. for up to six qubits. However, to investigate this correlation we needed an independent way to gauge the amount of entanglement of a state and in order to do so we improved existing numerical methods to determine the distance of a state to the set of separable symmetric states, using a combination of linear and quadratic programming. The tensor representation of symmetric multi-qubit states was also used to formally define a new tensor class of regularly decomposable tensors that corresponds to the set of separable symmetric multi-qubit states.

1.2. Français

Le thème central de cette thèse cumulative est l'étude de l'intrication multi-partite quantique pour des systèmes de dimension finie. Nous avons développé un algorithme numérique basé sur un problème d'optimisation semi-définie, qui permet de décider si un état est intriqué ou pas en un nombre fini d'itérations. Cet algorithme est une extension d'algorithmes déjà connus qui ne permettent pas de conclure lorsque l'état en question est séparable. Dans notre cas, si l'état est séparable, l'algorithme permet d'obtenir une décomposition de l'état en une mixture d'états séparables. Ces résultats ont été obtenus en exploitant la correspondance entre le problème de l'intrication et le problème des moments tronqués (truncated moment problem). Nous avons aussi développé une nouvelle manière d'exprimer l'état partiellement transposé d'un état symétrique de plusieurs qubits, simplifiant par la-même nombre de résultats bien connus en théorie de l'intrication. Cette nouvelle manière d'écrire le critère de transposée partielle unifie différentes interprétations et formulations alternatives dudit critère, et fait partie intégrante de notre algorithme d'optimisation semi-définie.

Nous avons aussi étudié en détails les propriétés géométriques des états intriqués de deux qubits : nous avons pu répondre à la question de savoir à quelle distance un état pur est de l'enveloppe convexe des états symétriques et séparables, en donnant une formule explicite de l'état symétrique et séparable le plus proche — la distance étant celle de Hilbert-Schmidt. Pour les états mixtes nous avons pu obtenir et une borne supérieure numérique et une borne inférieure analytique pour cette distance. Pour un plus grand

nombre de qubits, nous nous sommes intéressés à la boule des états absolument classique, c'est à dire des états symétriques de plusieurs qubits qui restent séparables sous n'importe quelle transformation unitaire. Nous avons trouvé une borne inférieure analytique pour le rayon de cette boule autour de l'état maximallement mixte ainsi qu'une borne supérieure numérique, cette dernière ayant été obtenue en cherchant un état intriqué aussi proche que possible de l'état maximallement mixte.

La représentation tensorielle d'un état symétrique de plusieurs qubits, autrement dit de l'état d'un spin j , nous a permis d'étudier des propriétés de l'intrication en nous basant sur le spectre du tenseur (valeurs propres du tenseur). Le caractère défini du tenseur est relié à l'intrication de l'état qu'il représente, donnant la possibilité de détecter la présence d'intrication à l'aide de la valeur propre minimale du tenseur. Toutefois, les valeurs propres du tenseur sont autrement plus compliquée à calculer que les valeurs propres matricielle, rendant l'analyse numérique plus délicate. La relation entre la valeur propre minimale du tenseur et la quantité d'intrication présente dans l'état a aussi été étudiée. Il en ressort que les deux quantités sont étroitement corrélées pour des systèmes de petite taille, c'est à dire jusqu'à six qubits. L'étude de ces corrélations a nécessité une méthode indépendante pour jauger de la quantité d'intrication présente dans un état. Pour cela nous avons amélioré des méthodes numériques pour déterminer la distance entre un état et l'ensemble composé des états symétriques et séparables, en utilisant une combinaison d'algorithmes d'optimisation quadratique et d'optimisation linéaire. La représentation tensorielle des états symétriques de plusieurs qubits a aussi été utilisée pour définir formellement une nouvelle classe de tenseurs, appelés "regularly decomposable tensors", qui correspond à l'ensemble des états symétriques et séparables de plusieurs qubits.

1.3. Deutsch

Das zentrale Thema dieser kumulativen Dissertation ist die Untersuchung der multipartiten Quantenverschränkung endlich dimensionaler Systeme. Wir entwickelten einen semidefiniten Optimisierungsalgorithmus der in einer endlichen Anzahl von Schritten erkennt, ob ein Zustand separabel oder verschränkt ist. Dieser Algorithmus ist eine Erweiterung von bestehenden semidefiniten Methoden, die keine Aussage treffen, wenn der Zustand separabel ist. Wir hingegen sind in der Lage in diesem Fall eine explizite Zerlegung in ein Gemisch aus reinen separablen Zuständen auszugeben. Dies erreichten wir indem wir das Verschränkungsproblem als mathematisches „truncated moment problem“ umschreiben, für welches es wiederum existierende numerische Lösungsmethoden gibt.

Darüber hinaus entwickelten wir eine neue Art das partielle Transpositionskriterium zu formulieren, wodurch wir in der Lage waren einige existierende Verschränkungskriterien zu vereinen. Diese Reformulierung wird auch in dem neu entwickelten numerischen Algorithmus genutzt.

Die geometrischen Eigenschaften von symmetrischen zwei Qubit Zuständen wurden detailliert untersucht. Wir konnten die Frage beantworten, wie weit ein reiner Zustand von der konvexen Hülle der separablen symmetrischen Zuständen entfernt liegt. Außerdem konnten wir für gemischte Zustände eine analytische untere Schranke und eine numerische obere Schranke für diese Entfernung angeben. Für größere Qubitsysteme untersuchten wir den Ball der absolut klassischen Zustände, d.h. der symmetrischen Vielteilchen-Qubit Zustände, die unter jeder unitären Transformation separable bleiben. Für den Radius dieses Balles um den maximal gemischten Zustand fanden wir eine analytische untere Schranke; außerdem konnten wir eine numerische obere Schranke angeben, indem wir nach einem verschränkten Zustand gesucht haben der sich so nah wie möglich an dem maximal gemischten Zustand befindet.

Die Tensor-Darstellung von symmetrischen Vielteilchen-Qubit Zuständen, oder auch Spin- j Zuständen, erlaubte uns Verschränkungseigenschaften mit dem Spektrum eines Tensors in Verbindung zu bringen, indem wir Tensoreigenwerte untersuchten. Die Definitheit dieses Tensors steht im Verhältnis zu der Verschränkung des zugrunde liegenden Zustandes und daher kann der kleinste Tensoreigenwert genutzt werden um Verschränkung zu detektieren. Allerdings sind Tensoreigenwerte komplizierter zu berechnen als die üblichen Matrixeigenwerte, was diese Untersuchung erschwerte. Darüber hinaus untersuchten wir auch das Verhältnis zwischen dem Wert des kleinsten Tensoreigenwerts und der Quantität der Verschränkung. Es stellte sich heraus, dass diese zwei für kleine Systeme von bis zu sechs Qubits stark korreliert sind. Für diese Untersuchung benötigten wir allerdings eine unabhängige Methode um die Verschränkungsstärke zu messen, daher entwickelten wir eine bekannte Methode weiter, die den minimalen Hilbert-Schmidt Abstand zu den separablen symmetrischen Zuständen bestimmt. Dies wurde durch eine Kombination aus einem linearen und einem quadratischen Programm erreicht. Die Tensor-Darstellung wurde auch genutzt um eine neue Klasse von "regulär zerlegbaren Tensoren" formal zu definieren, die exakt der Menge der separablen symmetrischen Zuständen entspricht.

2. Spin states

In this chapter we will introduce spin coherent states and related concepts, which are essential ingredients in the publications of this thesis. The presentation will be more detailed than in the papers to help readers who are not familiar with those concepts and to provide a sound background to understand the more compact descriptions in the publications. The descriptions in this chapter are based on the book [1].

2.1. Spin- j states

The theory of spin states can be started with the generators of rotation around the i -th axes J_i , which obey the fundamental commutator relations

$$[J_i, J_j] = i\epsilon_{ijk}J_k, \quad i, j, k \in \{1, 2, 3\}, \quad (2.1)$$

with ϵ_{ijk} the Levi-Civita symbol. We take $\hbar = 1$ throughout this thesis and use as label for the axes either letters as in J_x, J_y, J_z or equivalently numbers as in J_1, J_2, J_3 . Since the three J_i operators do not commute a basis of all spin- j states cannot be given only by eigenstates of the J_i operators. Instead we will also use the operator

$$\mathbf{J}^2 \equiv \mathbf{J} \cdot \mathbf{J} = J_x^2 + J_y^2 + J_z^2, \quad (2.2)$$

which commutes with all J_i , as

$$[\mathbf{J}^2, J_i] = 0 \quad \forall i. \quad (2.3)$$

Therefore, any spin state can be written in the basis $|j, m\rangle$ of common eigenstates of \mathbf{J}^2 and e.g. J_z with

$$\mathbf{J}^2 |j, m\rangle = j(j+1) |j, m\rangle, \quad j = \frac{n}{2}, n \in \mathbb{N} \quad (2.4)$$

$$J_z |j, m\rangle = m |j, m\rangle, \quad m \in \{-j, \dots, j\}. \quad (2.5)$$

The rotation operator around the normalized vector \mathbf{n} with the rotation angle ϕ can be written with the generators of rotation defined by (2.1) as

$$R_j(\mathbf{n}, \phi) = e^{-i\phi \mathbf{J} \cdot \mathbf{n}}. \quad (2.6)$$

From this definition it is obvious that a rotation cannot change the value of j because \mathbf{J}^2 commutes with every J_k and hence also with functions of it.

For computational aid we define the ladder operators as

$$J_{\pm} = J_x \pm iJ_y. \quad (2.7)$$

These non-Hermitian operators obey the commutation relations

$$[J_+, J_-] = 2J_z, \quad [J_z, J_{\pm}] = \pm J_{\pm}, \quad \text{and} \quad [\mathbf{J}^2, J_{\pm}] = 0, \quad (2.8)$$

which can be worked out with (2.3). These ladder operators have the property that they raise or lower the quantum number m , as

$$J_{\pm} |j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)} |j, m \pm 1\rangle, \quad (2.9)$$

which can be derived with (2.8).

2.2. Spin coherent states

Spin coherent states can be defined as the eigenstates of the vector spin operator with eigenvalue j , such that

$$\mathbf{J} \cdot \mathbf{n} |\alpha\rangle = j |\alpha\rangle, \quad (2.10)$$

with $\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T$, where T stands for the transposition.

To find all states of this form we start by guessing a state that fulfills (2.10), which is the spin-up state $|j, j\rangle$, and $\mathbf{n} = (0, 0, 1)^T$ such that

$$J_z |j, j\rangle = j |j, j\rangle. \quad (2.11)$$

With that solution we can generate all states of the form (2.10) by rotating the state $|j, j\rangle$ around the y-axes and then the z-axes with angles θ and ϕ [we define the compact

notation $\alpha = (\theta, \phi)$ such that θ is the polar angle and ϕ the azimuthal angle, as

$$\boxed{|\alpha\rangle = R_j(\theta, \phi) |j, j\rangle = e^{-i\phi J_z} e^{-i\theta J_y} |j, j\rangle.} \quad (2.12)$$

All rotated states of $|j, j\rangle$ can be reached in this way. All states of this form satisfy (2.10), which can be seen by a direct calculation of

$$R_j(\theta, \phi)^\dagger (\mathbf{J} \cdot \mathbf{n}) R_j(\theta, \phi) = J_z \quad (2.13)$$

or intuitively by rotating the coordinate system. With this definition of spin coherent states it is obvious that they remain coherent under rotation, since only the angles (θ, ϕ) will change.

For practical applications it is useful to write the spin coherent state in the usual $|j, m\rangle$ basis. This calculation will be worked out here in detail. First we insert the identity operator in the $|j, m\rangle$ basis to get

$$\begin{aligned} |\alpha\rangle &= \sum_{m=-j}^j |j, m\rangle \langle j, m| e^{-i\phi J_z} e^{-i\theta J_y} |j, j\rangle \\ &= \sum_{m=-j}^j e^{-im\phi} |j, m\rangle \langle j, m| e^{-i\theta J_y} |j, j\rangle, \end{aligned} \quad (2.14)$$

where we have used $\langle j, m| e^{-i\phi J_z} = e^{-im\phi} \langle j, m|$ by Eq. (2.5). That leaves the calculation of

$$d_m(\theta) = \langle j, m| e^{-i\theta J_y} |j, j\rangle, \quad (2.15)$$

which is a special case of the general Wigner d-matrix [2]. To derive the explicit form of $d_m(\theta)$, we will introduce Schwinger's oscillator model.

2.2.1. Schwinger's oscillator model

Schwinger's oscillator model [3] connects a spin- j state to the state of two uncoupled harmonic oscillators with a total number of $2j$ excitations, such that the description is formally equivalent.

The first harmonic oscillator will be labeled with a plus and the second with a minus sign. The usual commutation relations between the creation and annihilation operators

apply,

$$[a_+, a_+^\dagger] = 1, \quad [a_-, a_-^\dagger] = 1, \quad (2.16)$$

where a_+ (a_-) is the annihilation operator of the plus (minus) type oscillator.

The harmonic oscillators are separated physical systems and therefore

$$[a_+, a_-^\dagger] = [a_-, a_+^\dagger] = 0. \quad (2.17)$$

All number states of the harmonic oscillators can be generated from the ground state of both oscillators defined by $a_\pm |0, 0\rangle = 0$ by

$$\left(a_+^\dagger\right)^{n_+} \left(a_-^\dagger\right)^{n_-} |0, 0\rangle = \sqrt{n_+! n_-!} |n_+, n_-\rangle, \quad n_+, n_- \in \mathbb{N}. \quad (2.18)$$

With those operators one can then define

$$J_z \equiv \frac{a_+^\dagger a_+ - a_-^\dagger a_-}{2}, \quad J_+ \equiv a_+^\dagger a_-, \quad J_- \equiv a_-^\dagger a_+. \quad (2.19)$$

It is easy to see that these operators satisfy the angular momentum commutation relations (2.8) and are therefore formally equivalent to angular momentum operators. The application of J_+ destroys one excitation in the minus-type oscillator and creates one in the plus-type. Hence, just like the action of the ladder operator given in (2.7), the action of J_+ corresponds to an increase of the spin quantum number m by one. The operator J_- does the opposite action, while the J_z counts the difference between the two occupation numbers of both oscillators. This allows to make the connection

$$j = \frac{n_+ + n_-}{2}, \quad m = \frac{n_+ - n_-}{2}, \quad (2.20)$$

where n_+ (n_-) is the number of photons in the plus (minus) type oscillator, given as

$$a_\pm^\dagger a_\pm |n_+, n_-\rangle = n_\pm |n_+, n_-\rangle. \quad (2.21)$$

This allows us to make the identification

$$|j, m\rangle = \frac{\left(a_+^\dagger\right)^{j+m} \left(a_-^\dagger\right)^{j-m}}{\sqrt{(j+m)!(j-m)!}} |0, 0\rangle, \quad (2.22)$$

where $|0, 0\rangle$ is the again the ground state of both harmonic oscillators. With that a spin- j state can be visualized as being a symmetric state of $2j$ bosonic spin-1/2 particles, with $(j + m)$ of them pointing upwards and $(j - m)$ pointing downwards.

In the process of calculating the expression (2.15) we will further use the operator

$$J_y = \frac{a_+^\dagger a_- - a_-^\dagger a_+}{2i}, \quad (2.23)$$

which is derived from $J_y = \frac{1}{2i}(J_+ - J_-)$ and the state

$$|j, j\rangle = \frac{(a_+^\dagger)^{2j}}{\sqrt{(2j)!}} |0, 0\rangle. \quad (2.24)$$

2.2.2. Wigner's d-Matrix

Using this connection allows to utilize (2.23) and (2.24) to write

$$d_m(\theta) = \frac{1}{\sqrt{(2j)!}} \langle j, m | e^{-i\theta J_y} (a_+^\dagger)^{2j} e^{i\theta J_y} \underbrace{e^{-i\theta J_y} |0, 0\rangle}_{|0, 0\rangle}, \quad (2.25)$$

where the identification in the underbracket is correct since the operator J_y (2.23) acts always first with an annihilation operator, so only the first term in the expansion of the exponential function, $\mathbb{1}$, contributes. By repeatedly inserting identities in the form of $e^{i\theta J_y} e^{-i\theta J_y}$ in between the products of a_+^\dagger , Eq. (2.25) can be written as

$$d_m(\theta) = \frac{1}{\sqrt{(2j)!}} \langle j, m | \left(e^{-i\theta J_y} a_+^\dagger e^{i\theta J_y} \right)^{2j} |0, 0\rangle. \quad (2.26)$$

Using the Baker-Campbell-Hausdorff formula, the bracket in (2.26) can be calculated as

$$e^{-i\theta J_y} a_+^\dagger e^{i\theta J_y} = \sum_{k=0}^{\infty} \frac{(i\theta)^k}{k!} [J_y, a_+^\dagger]_k \quad (2.27)$$

with the commutator function defined as

$$[A, B]_0 = B, \quad \text{and} \quad [A, B]_k = [A, [A, B]_{k-1}]. \quad (2.28)$$

Next, we calculate the commutator function appearing in the sum by using Eq. (2.23) and obtain for

$$[J_y, a_+^\dagger] = -\frac{1}{2i}[a_-^\dagger a_+, a_+^\dagger] = -\frac{1}{2i}a_-^\dagger, \quad (2.29)$$

and

$$[J_y, a_-^\dagger] = \frac{1}{2i}[a_+^\dagger a_-, a_-^\dagger] = \frac{1}{2i}a_+^\dagger. \quad (2.30)$$

With these two results we get the general form, as

$$[J_y, a_\pm^\dagger]_k = \begin{cases} 2^{-k}a_\pm^\dagger & k \text{ even} \\ i2^{-k}a_\mp^\dagger & k \text{ odd.} \end{cases} \quad (2.31)$$

Now, inserting (2.31) into Eq.(2.27) and sorting the sum into even and odd parts gives

$$\sum_{k=0}^{\infty} \frac{(i\theta)^k}{k!} [J_y, a_+^\dagger]_k = \sum_{k=0}^{\infty} \left\{ \frac{(-1)^k}{(2k)!} \left(\frac{\theta}{2}\right)^{2k} a_+^\dagger - \frac{(-1)^k}{(2k+1)!} \left(\frac{\theta}{2}\right)^{2k+1} a_-^\dagger \right\} \quad (2.32)$$

$$= \cos\left(\frac{\theta}{2}\right) a_+^\dagger - \sin\left(\frac{\theta}{2}\right) a_-^\dagger. \quad (2.33)$$

This result is now inserted into Eq. (2.26), as

$$d_m(\theta) = \frac{1}{\sqrt{(2j)!}} \langle j, m | \left[\cos\left(\frac{\theta}{2}\right) a_+^\dagger - \sin\left(\frac{\theta}{2}\right) a_-^\dagger \right]^{2j} | 0, 0 \rangle. \quad (2.34)$$

Because the operators of the plus and the minus type commute, we can use the binomial formula and apply it to the zero state, as

$$d_m(\theta) = \frac{1}{\sqrt{(2j)!}} \langle j, m | \sum_{k=0}^{2j} \binom{2j}{k} \cos\left(\frac{\theta}{2}\right)^{2j-k} \sin\left(\frac{\theta}{2}\right)^k (a_+^\dagger)^{2j-k} (a_-^\dagger)^k | 0, 0 \rangle \quad (2.35)$$

$$= \frac{1}{\sqrt{(2j)!}} \sum_{k=0}^{2j} \binom{2j}{k} \cos\left(\frac{\theta}{2}\right)^{2j-k} \sin\left(\frac{\theta}{2}\right)^k \sqrt{(2j-k)!} \sqrt{k!} \langle j, m | j, j-k \rangle, \quad (2.36)$$

$$(2.37)$$

where we have used (2.22) to get $|j, j - k\rangle$. The orthonormality of the $|j, m\rangle$ basis allows to identify $\langle j, m | j, j - k \rangle = \delta_{m, j-k} = \delta_{k, j-m}$, and thus

$$d_m(\theta) = \frac{1}{\sqrt{(2j)!}} \binom{2j}{j-m} \sqrt{(j+m)!} \sqrt{(j-m)!} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2}\right)^{j-m} \quad (2.38)$$

$$= \sqrt{\binom{2j}{j+m}} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2}\right)^{j-m}. \quad (2.39)$$

Now, we can finally insert this into Eq. (2.14) to get the explicit form of a spin coherent state in the $|j, m\rangle$ basis as

$$|\alpha\rangle = \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2} e^{i\phi}\right)^{j-m} |j, m\rangle, \quad (2.40)$$

where the state was multiplied with an irrelevant phase factor $e^{ij\phi}$. Note that in the literature there is no agreement on the conventions of the signs of the angles θ and ϕ .

2.3. Properties of spin coherent states

In this section we will discuss some properties of spin coherent states. In the following we will use two different names for two-level states, either spins-1/2 states if we talk about a single system, or **qubits** if we consider multi-partite states of many two-level systems.

2.3.1. Spin- j states as combination of qubits

By the rules of addition of angular momentum, a N qubit symmetric state can be seen as a spin- j state, with $j = N/2$, if the qubits are added to a maximal total spin of j . This can be seen easily by acting with the ladder operator $J_- = J_x - iJ_y$ on the state $|j, j\rangle$, where this state can be created by adding N times the qubit up-state, as $|\frac{1}{2}, \frac{1}{2}\rangle^{\otimes N}$ in the Hilbert space of N qubits. Note that one can use the operator J_- to go from one basis state to another, as

$$J_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} |j, m-1\rangle. \quad (2.41)$$

So by repeatedly applying J_- to $|j, j\rangle$ one can generate all basis states $|j, m\rangle$. Because both $|j, j\rangle$ and J_- are fully symmetric under the permutation of all qubits, all $|j, m\rangle$

states also lie in the fully symmetric subspace of the total Hilbert space $\mathcal{H} = \mathbb{C}^{2^N}$ of N -qubits.

The explicit form of the spin- j states $|j, m\rangle$ in the Hilbert space of N -qubits $\mathcal{H} = \mathbb{C}^{2^N}$, is given as the **Dicke state** [4]

$$\left|D_N^{(k)}\right\rangle = \mathcal{N} \sum_{\pi} \underbrace{|\uparrow \dots \uparrow\rangle}_k \underbrace{|\downarrow \dots \downarrow\rangle}_{N-k}, \quad k = 0, \dots, N, \quad (2.42)$$

where the sum runs over all permutations of the the qubits, written here as $|\uparrow\rangle \equiv \left|\frac{1}{2}, \frac{1}{2}\right\rangle$ and $|\downarrow\rangle \equiv \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, and with \mathcal{N} a normalization constant.

Then we have the correspondence

$$|j, m\rangle \leftrightarrow \left|D_{2j}^{(j+m)}\right\rangle, \quad (2.43)$$

since in the state $\left|D_{2j}^{(j+m)}\right\rangle$, $(j+m)$ qubits point upwards each of them give a contribution of $\frac{1}{2}$ to m , and the remaining $(j-m)$ qubits point downwards which give each a contribution of $-\frac{1}{2}$ to m . So the value of m is indeed

$$\frac{1}{2}(j+m) - \frac{1}{2}(j-m) = m. \quad (2.44)$$

With that correspondence, we see that spin- j coherent states have a particular simple decomposition as a multi-qubit state, since they can be written as tensor product of identical qubit states as

$$|\alpha\rangle_j = \underbrace{|\alpha\rangle_{\frac{1}{2}} \otimes \dots \otimes |\alpha\rangle_{\frac{1}{2}}}_{2j} \quad (2.45)$$

where we have added a subscript indicating the total spin quantum number and we denote a pure qubit state as $|\alpha\rangle_{\frac{1}{2}}$, since all pure qubit states are also spin-1/2 coherent states. This identification can be seen by direct calculation or more easily with the definition of spin coherent states (2.12): The state $|j, j\rangle$ can be written as the $2j$ -fold tensor product of the qubit state $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ and the rotation of the state $|j, j\rangle$ can be written

as identical rotations on the individual qubit states, as

$$|\alpha\rangle_j = R_j(\theta, \phi) |j, j\rangle = \underbrace{R_{1/2}(\theta, \phi) \left| \frac{1}{2}, \frac{1}{2} \right\rangle \otimes \cdots \otimes R_{1/2}(\theta, \phi) \left| \frac{1}{2}, \frac{1}{2} \right\rangle}_{2j} \quad (2.46)$$

$$= \underbrace{|\alpha\rangle_{\frac{1}{2}} \otimes \cdots \otimes |\alpha\rangle_{\frac{1}{2}}}_{2j}, \quad (2.47)$$

where $R_j(\theta, \phi)$ is a rotation of a spin- j state and $R_{1/2}(\theta, \phi)$ is a rotation of a single qubit.

Until here we have only talked about symmetric pure states. If also symmetric mixed states are considered, the situation becomes more subtle. A mixed symmetric state of qubits is a classical mixture of pure symmetric states $|\psi_i\rangle_{\text{sym}}$ as

$$\rho = \sum_i w_i |\psi_i\rangle_{\text{sym}} \langle \psi_i|_{\text{sym}}, \quad (2.48)$$

with $\sum_i w_i = 1$ and $w_i > 0$. This definition implies that a symmetric state is equal to its projection onto the symmetric subspace spanned by the Dicke states. It is important to stress that for mixed states it is not enough to demand that a state should be invariant under permutations of the subsystems, since this can also be achieved by classical symmetrization. We want to consider only a symmetry which originates in the quantum nature of indistinguishable particles. To make this distinction clear we will give an example of a state which is not symmetric in this sense. Consider the state

$$\rho = \sigma \otimes \sigma \quad (2.49)$$

with σ a non-pure qubit state. This state is not a symmetric state, which can be seen by writing σ as a decomposition of two pure qubit states

$$\sigma = w |\psi\rangle \langle \psi| + (1 - w) |\phi\rangle \langle \phi|. \quad (2.50)$$

Then

$$\rho = w^2 |\psi\psi\rangle \langle \psi\psi| + (1 - w)^2 |\phi\phi\rangle \langle \phi\phi| + w(1 - w)(|\psi\phi\rangle \langle \psi\phi| + |\phi\psi\rangle \langle \phi\psi|), \quad (2.51)$$

where the last two contributions are not symmetric, i.e. the projection onto the anti-symmetric singlet state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is in general (for $|\phi\rangle \neq |\psi\rangle$ and $1 > w > 0$)

not zero:

$$\langle \Psi | \rho | \Psi \rangle = 2w(1-w) |\langle \Psi | \psi \phi \rangle|^2 \neq 0. \quad (2.52)$$

Therefore the projection of ρ onto the Dicke states does not reproduce ρ . This is a subtle point as the classical uncertainty in the mixed state σ prevents the state ρ to be symmetric. Or in other words, every mixed symmetric state is invariant under permutation of the subsystems, but the reverse is, in general, not true.

2.3.2. Overlap of spin coherent states

The spin coherent states form an overcomplete basis of the $(2j+1)$ dimensional Hilbert space of spin- j states as,

$$\frac{2j+1}{4\pi} \int |\alpha\rangle \langle \alpha| d\alpha = \mathbb{1}_{2j+1}. \quad (2.53)$$

However, they are in general not orthogonal to each other. This can be seen by calculating the overlap of two different spin coherent states, with the explicit form (2.40) and the orthonormality of the $|j, m\rangle$ basis, as

$$\langle \alpha' | \alpha \rangle = \left(\cos \frac{\theta}{2} \cos \frac{\theta'}{2} + e^{i(\phi-\phi')} \sin \frac{\theta}{2} \sin \frac{\theta'}{2} \right)^{2j}, \quad (2.54)$$

which is in general not zero. The only states which are orthogonal to each other are the spin coherent states which lay at antipodal points on the sphere. This can be seen by calculating the absolute value of (2.54), as

$$\begin{aligned} |\langle \alpha' | \alpha \rangle| &= \left[\frac{1 + \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos (\phi - \phi')}{2} \right]^{2j} \\ &= \cos^{2j} \left(\frac{\beta}{2} \right), \end{aligned} \quad (2.55)$$

with β the angle between the two vectors $\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T$ and $\mathbf{n}' = (\sin \theta' \cos \phi', \sin \theta' \sin \phi', \cos \theta')^T$. Therefore Eq. (2.55) can only be zero if $\beta = \pi$, i.e. if the spin coherent states point in opposite directions.

2.3.3. Minimal uncertainty states

The spin coherent states are the states which have a minimal quantum uncertainty [5]. One possible uncertainty relation for spin states, which is invariant under $SU(2)$, reads

$$j \leq \Delta J_x^2 + \Delta J_y^2 + \Delta J_z^2 = \langle \mathbf{J}^2 \rangle - \sum_{k=1}^3 \langle J_k \rangle \langle J_k \rangle \leq j(j+1) \quad (2.56)$$

with

$$\Delta J_k^2 = \langle J_k^2 \rangle - \langle J_k \rangle^2. \quad (2.57)$$

The upper bound can be reached by rotating Eq.(2.56) into

$$\langle \mathbf{J}^2 \rangle - \langle J_z \rangle^2 \quad (2.58)$$

and then choosing a state which has a zero expectation value of J_z , and by noting that $\langle \mathbf{J}^2 \rangle = j(j+1)$ for all spin- j states. With the same argument the lower bound can be reached by states that have the maximal value j as expectation value of J_z .

This is exactly the case for all spin coherent states, as the uncertainty relation (2.56) gives

$$\langle \alpha | \mathbf{J}^2 | \alpha \rangle - \langle \alpha | \mathbf{J} | \alpha \rangle^2 = j(j+1) - j^2 = j, \quad (2.59)$$

where the first expectation value comes from Eq. (2.4) and the second from Eq. (2.10).

In this sense the spin coherent states are the states which point as much as possible in a well-defined direction, as

$$\langle \alpha | \mathbf{J} | \alpha \rangle = j \mathbf{n}. \quad (2.60)$$

This property is in general not fulfilled for an arbitrary spin- j state, if j is larger than one half, even if the state is pure: E.g. the state $|1, 0\rangle$ points nowhere.

2.4. Visualization of spin states

It is often elucidating to have an easy visual representation of a quantum state to get an intuition of its properties. One well known visualization of a spin-1/2 state is the Bloch ball which we will describe in the following.

2.4.1. Bloch Sphere

Any spin-1/2 state, i.e. a state of a two-level system can be written in the $|j, m\rangle$ basis as

$$|\psi\rangle = \cos \frac{\theta}{2} \left| \frac{1}{2}, \frac{1}{2} \right\rangle + e^{i\phi} \sin \frac{\theta}{2} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (2.61)$$

since the angles (θ, ϕ) give all possible linear combinations of the two basis states (modulus a global phase). This equates to the definition of the spin coherent states (2.40) with $j = \frac{1}{2}$. Therefore all pure qubit states are spin coherent states.

By using the vector $\mathbf{v} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T$ the two angles can be mapped to a vector of length one which represents any pure spin-1/2 state. This vector is called **Bloch vector**. As we have seen in Eq.(2.60) this vector gives the direction in which the state $|\psi\rangle$ points.

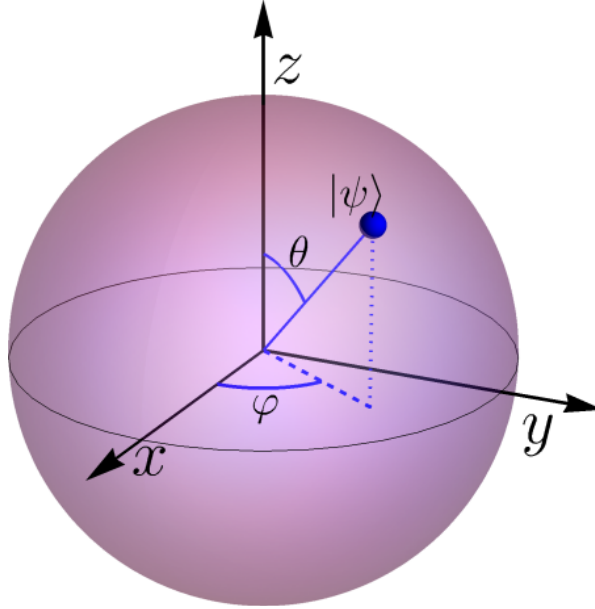


Figure 2.1.: The Bloch vector of a pure state $|\psi\rangle$. This state is represented by a Bloch vector with length one.

In the case of spin-1/2 states this concept is also valid for mixed states, as the Bloch vector can visualize any mixed spin-1/2 state, with a Bloch vector of length smaller than one. This can be seen by writing the 2×2 density matrix of a spin-1/2 state ρ in the basis of the \mathbf{J} operator, i.e. one half times the three Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2.62)$$

and the 2×2 identity matrix as,

$$\rho = \frac{1}{2} (\mathbb{1} + v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3). \quad (2.63)$$

Any qubit state, pure or mixed, can be written in this form. Just as in the case of pure states the entries of the Bloch vector can be determined by,

$$\mathbf{v} = \text{tr} \{ \rho \boldsymbol{\sigma} \}. \quad (2.64)$$

A crucial property of the Bloch vector is its behavior under rotation of the qubit state. If the state is rotated with U a $SU(2)$ -rotation operator into $\rho' = U\rho U^\dagger$, the corresponding Bloch vector \mathbf{v}' of ρ' is obtained by rotation of the original Bloch vector, namely $\mathbf{v}' = R\mathbf{v}$, with R the $O(3)$ rotation matrix which corresponds to the same rotation angle and rotation axes as the unitary operator U .

2.4.2. Majorana Representation

For values of j larger than $1/2$ the Bloch vector can be generalized to a tensor of $2j$ -indices [6] which behaves similarly under rotation as the Bloch vector and which has a particular simple form for spin coherent states. However, this so called Bloch tensor does not have a simple visual interpretation.

For this task we will introduce the Majorana representation, which gives an easy graphical picture of an arbitrary pure spin- j state [7]. Any spin- j state $|\psi\rangle$ can be written as

$$|\psi\rangle = \mathcal{N} \sum_{\pi} \{ |\chi_1\rangle \otimes |\chi_2\rangle \otimes \cdots \otimes |\chi_{2j}\rangle \}, \quad (2.65)$$

where the sum runs over all permutations of the $2j$ qubit states $|\chi_k\rangle$ and \mathcal{N} corresponds to the normalization factor. Each of these qubit states $|\chi_k\rangle$ has a Bloch vector \mathbf{v}_k , with length one, and therefore defining $2j$ points on the Bloch sphere. These points are called Majorana-stars [8]. (Note that in the original definition the Majorana stars are on the opposite side of the sphere, i.e. at $-v_k$)

However, transforming a given state into the form of Eq.(2.65) is not trivial. It can be achieved by exploiting the fact that antipodal spin coherent states are orthogonal to each other, as shown in (2.55). So one can calculate the overlap of the state with a spin coherent state $\langle \alpha' |_j$ written as the tensor product of identical qubit states as in (2.45).

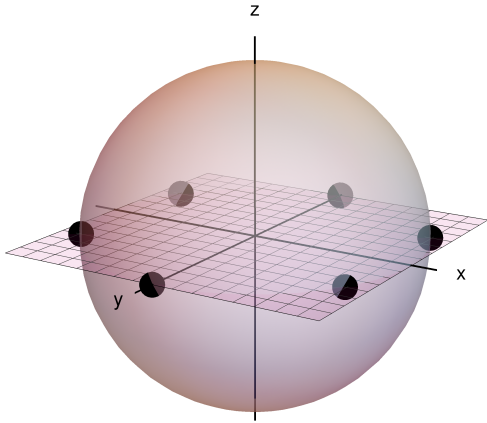


Figure 2.2.: The Majorana representation of the spin-3 state $\frac{1}{\sqrt{2}}(|3, 3\rangle + |3, -3\rangle)$ in the $|j, m\rangle$ notation. Black balls indicate the positions of the Majorana stars.

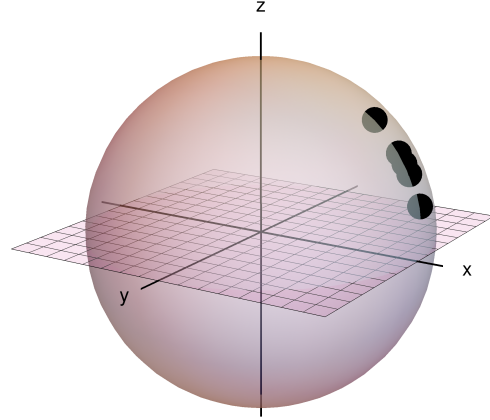


Figure 2.3.: The Majorana representation of the spin-5/2 state $\frac{1}{\sqrt{2}}(|\alpha_1\rangle + |\alpha_2\rangle)$, i.e. the superposition of two spin coherent states as in (2.40), with $\alpha_1 = (\theta = \frac{\pi}{3}, \phi = 0)$ and $\alpha_2 = (\theta = \frac{\pi}{3}, \phi = \frac{1}{5})$.

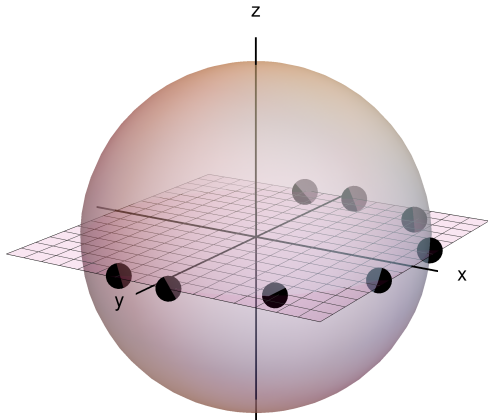


Figure 2.4.: The Majorana representation of the spin-4 state $\frac{1}{3} \sum_{m=-4}^4 |4, m\rangle$ in the $|j, m\rangle$ notation.

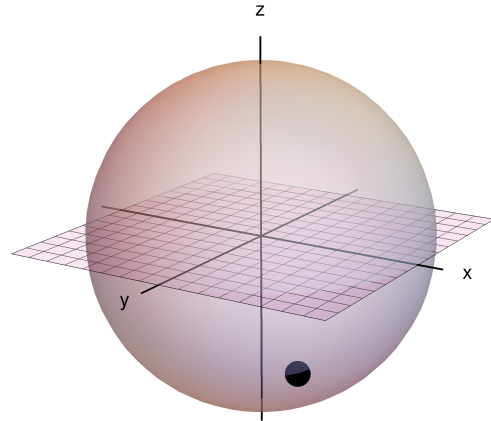


Figure 2.5.: The Majorana representation of the spin coherent state $|\alpha\rangle$ with $\alpha = (\theta = \frac{2\pi}{3}, \phi = \frac{7\pi}{4})$. This visualization is independent of j , since all $2j$ -points coincide.

The angle of the spin coherent state $\langle\alpha'|\alpha\rangle$ is chosen to be $\alpha' = (\theta + \pi, \phi)$ so that the spin coherent state is on the opposite side of the sphere in comparison with the usual definition $\langle\alpha|\alpha\rangle$ in Eq. (2.40).

Then, each of the identical qubit states $\langle \alpha' |_{1/2}$ gets multiplied with the $|\chi_k\rangle$ in (2.65):

$$\langle \alpha' | \psi \rangle \propto \langle \alpha' | \chi_1 \rangle_{1/2} \langle \alpha' | \chi_2 \rangle_{1/2} \cdots \langle \alpha' | \chi_{2j} \rangle_{1/2} \quad (2.66)$$

$$= \prod_{k=1}^{2j} \langle \alpha' | \chi_k \rangle_{1/2} \quad (2.67)$$

This product defines a polynomial of degree $2j$ in a single complex variable given by $\hat{\alpha}'$. This polynomial can then be decomposed as

$$\langle \alpha' | \psi \rangle \propto \prod_{k=1}^{2j} (\hat{\alpha}' - \hat{\chi}_k), \quad (2.68)$$

where $\hat{\chi}_k$ are its complex roots. These roots define exactly the position of the Majorana stars.

This can be intuitively understood in the sense that the spin coherent state $\langle \alpha' |$ scans which qubit contributions are present in the state $|\psi\rangle$, because if a certain value of α' makes the polynomial vanish, the state $|\psi\rangle$ must have a contribution $|\chi_k\rangle$ which is antipodal to $|\alpha'\rangle$. Thus calculating all roots, with their multiplicity gives all the $|\chi_k\rangle$ in (2.65).

For an explicit calculation of these roots, Eq.(2.67) can be written with the state $|\psi\rangle = \sum_{m=-j}^j \psi_m |j, m\rangle$, as

$$\langle \alpha' | \psi \rangle \propto \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(-e^{-i\phi} \cot \frac{\theta}{2} \right)^{j-m} \psi_m \quad (2.69)$$

$$= \sum_{k=0}^{2j} \sqrt{\binom{2j}{k}} \left(-e^{-i\phi} \cot \frac{\theta}{2} \right)^{2j-k} \psi_{k-j} \quad (2.70)$$

$$= \sum_{k=0}^{2j} \sqrt{\binom{2j}{k}} \psi_{k-j} z^{2j-k}, \quad (2.71)$$

which has $2j$ roots in the complex variable $z = -e^{-i\phi} \cot \frac{\theta}{2}$. These roots can then be expressed with the angles (θ_k, ϕ_k) . If the state $|\psi\rangle$ is a spin coherent state itself, the polynomial has only a single root which is $2j$ -fold degenerated.

2.5. Entanglement and Quantumness

2.5.1. Classical spin states

Any spin- j state ρ can be expressed in the overcomplete basis of spin coherent states, with the Glauber-Sudarshan P-function [9, 10] as

$$\rho = \int P(\alpha) |\alpha\rangle \langle \alpha| d\alpha \quad (2.72)$$

with $d\alpha = \sin\theta d\theta d\phi$. The normalization of the state ρ gives the condition

$$\text{tr}\rho = \int P(\alpha) d\alpha = 1, \quad (2.73)$$

and the P-function can always be chosen as a real function.

Any state for which a positive P-function exists is called a **classical spin state** [11] and the set of classical spin states is denoted \mathcal{C} . This definition is reasonable since the P-function can be seen as a probabilistic mixture of spin coherent states, which in turn resemble a classical objects as close as possible.

If a spin- j state is classical it can be written as a decomposition over at most $(2j+1)^2$ spin coherent states as,

$$\rho = \sum_{k=1}^{(2j+1)^2} p_k |\alpha_k\rangle \langle \alpha_k|. \quad (2.74)$$

This can be derived by applying Carathéodory's theorem to the Hilbert space of a spin- j state, where one degree of freedom is removed due to the normalization of the state, $\text{tr}\rho = 1$. Therefore the question if a spin- j state is classical is equivalent to the question if there exists spin coherent states $|\alpha_k\rangle$ and numbers $p_k \geq 0$, with $\sum_k p_k = 1$, such that Eq. (2.74) holds.

With this definition of classical states one can ask which states are non-classical? A measure¹ of this non-classicality will be called **Quantumness** and defined [13] as,

$$Q(\rho) = \min_{\rho_c \in \mathcal{C}} \|\rho - \rho_c\| \quad (2.75)$$

¹The word "measure" is used here, not in the sense that this defines an entanglement measure, since it was shown that the Hilbert-Schmidt distance does not fulfill all axioms demanded from an entanglement measure [12].

where $\|A\| = \sqrt{\text{tr}(A^\dagger A)}$ is the Hilbert-Schmidt norm, and the minimization is performed over all classical states. So $Q(\rho)$ gives the Hilbert-Schmidt distance to the closest classical state and hence the state ρ is non-classical if and only if $Q(\rho) > 0$.

2.5.2. Separable states

Classicality or Quantumness, is a property defined for a spin- j state. However, if one sees a spin- j state as a symmetric multi-qubit state, as in (2.65), one can investigate how these concepts are viewed for a multi-partite state.

A pure state $|\psi\rangle$ in a Hilbert space is called **fully separable** if it can be written as a direct product of pure states of subsystems,

$$|\psi\rangle = |\psi^{(1)}\rangle \otimes \dots \otimes |\psi^{(N)}\rangle. \quad (2.76)$$

If a pure state cannot be written in this tensor product form it is called **entangled** [14]. For symmetric states every state which is not fully separable is automatically genuine full-partite entangled, i.e. all subsystems are entangled with all others, since all subsystems are interchangeable. Therefore the definition of entanglement is simpler if the state is a symmetric state of $2j$ qubit states, i.e. equivalent to a spin- j state.

We have seen in Eq.(2.45) that a spin coherent state $|\alpha\rangle$ can be written as tensor product of identical qubit states, each one pointing in the same direction as $|\alpha\rangle$. Therefore every spin coherent state is equivalent to a fully separable state of $2j$ -qubits. The converse is also true since any fully separable symmetric state of N qubits has to have all qubits identical and, since every pure qubit state is a spin coherent state, combining N of them gives a spin- $N/2$ coherent state.

These equivalences give an interesting connection between directionality and separability, in the sense that the counter intuitive picture of a spin without a direction corresponds to another genuine quantum feature: entanglement. This is directly visible with the Majorana representation: If the Majorana stars do not all coincide the equivalent multi-qubit state is entangled.

The definition of entanglement can be extended to mixed states. A mixed state is called fully separable if it can be written as

$$\rho = \sum_i w_i \rho_i^{(1)} \otimes \dots \otimes \rho_i^{(N)}, \quad (2.77)$$

with $\rho^{(k)}$ a state of the subsystem k , $\sum_i w_i = 1$ and $w_i \geq 0$. Now, if the separable mixed

state should also be symmetric, this restricts the definition further as a symmetric state can only be build by mixing pure symmetric states as shown in (2.48). Hence, a mixed symmetric separable state must be given by

$$\rho = \sum_i w_i \left| \chi_i^{(1)} \right\rangle \left\langle \chi_i^{(1)} \right| \otimes \cdots \otimes \left| \chi_i^{(N)} \right\rangle \left\langle \chi_i^{(N)} \right| \quad (2.78)$$

$$= \sum_i w_i \left| \chi_i^{(1)} \cdots \chi_i^{(N)} \right\rangle \left\langle \chi_i^{(1)} \cdots \chi_i^{(N)} \right|, \quad (2.79)$$

with the qubit pure states $\left| \chi_i^{(k)} \right\rangle = \left| \chi_i^{(k')} \right\rangle$, $\forall k, k', \sum_i w_i = 1$ and $w_i \geq 0$. The qubit states have to be all identical since otherwise the multi-qubit states may be entangled. Therefore the pure states in the decomposition (2.78) are equivalent to spin coherent states (2.45). So every separable mixed state is equivalent to a classical state (2.74). The other direction is obvious, since classically mixing separable states, i.e. spin coherent states, can only give a mixed separable state.

These equivalences are summarized in Table 2.1.

Table 2.1.: Connection between multi-qubit states and spin- j states

Spin- j	\leftrightarrow	Symmetric state of N qubits
spin coherent state $ \alpha\rangle$	\leftrightarrow	separable state $ \psi_{\text{sep}}\rangle = \psi^{(1)}\rangle \otimes \cdots \otimes \psi^{(N)}\rangle$
classical spin state $\rho = \int P(\alpha) \alpha\rangle \langle \alpha d\alpha$ with $P(\alpha) \geq 0$	\leftrightarrow	separable mixed state $\rho = \sum_i w_i \psi_{\text{sep}}\rangle_i \langle \psi_{\text{sep}} _i$ with $w_i \geq 0$

This identification allows to use tools designed to test for entanglement, e.g. the positive partial transpose criterion [15, 16], as a test for classicality. This criterion is defined for a bipartite state

$$\rho = \sum_{ijkl} p_{kl}^{ij} |i\rangle \langle j| \otimes |k\rangle \langle l|, \quad (2.80)$$

which acts on $\mathcal{H}^A \otimes \mathcal{H}^B$, as

$$\rho^{pt} = \sum_{ijkl} p_{lk}^{ij} |i\rangle \langle j| \otimes |k\rangle \langle l| \geq 0. \quad (2.81)$$

(Note the interchange in the index $l \leftrightarrow k$ in the coefficient p .) Here the partial transposition is performed on the second Hilbert space \mathcal{H}^B .

In the case of $j = 1$ a necessary and sufficient classicality criterion was derived in [11]

as,

$$Z_{ab} = \text{tr} \{ \rho (J_a J_b + J_b J_a) \} - \text{tr} \{ \rho J_a \} \text{tr} \{ \rho J_b \} - \delta_{a,b} \geq 0, \quad (2.82)$$

with $a, b \in \{1, 2, 3\}$ and J_a the spin-1 angular momentum operators. This criterion turns out to be just the positive partial transpose criterion in disguise, as the Z-matrix (2.82) is positive semi-definite if and only if the partial transposed density matrix of the corresponding two-qubit state is positive semi-definite. This can be seen by writing the partial transposed state of a symmetric two qubit state as [A.2],

$$2(U^\dagger \rho^{pt} U)_{a,b} = \text{tr} \{ \rho \sigma_a \otimes \sigma_b \} = T_{ab}, \quad (2.83)$$

with U a unitary matrix, $\sigma_0 = \mathbb{1}_2$, and $\sigma_{1,2,3}$ the three Pauli matrices. The right-hand-side is positive semi-definite if and only if the partial transposed state is positive semi-definite, because ρ^{pt} has the same eigenvalues up to a factor two as the matrix T .

A method to test if a d -dimensional matrix M is positive semi-definite is to calculate the Schur complement [17]. One special case of this method is with respect to the upper left corner M_{00} as,

$$S_{ab} = M_{ab} - M_{a0} M_{00}^{-1} M_{0b}, \quad a, b \in \{1, 2, \dots, d-1\}. \quad (2.84)$$

Then the matrix M is positive semi-definite if and only if $M_{00} \geq 0$ and S is positive semi-definite.

Applying this criterion to the matrix T with respect to the upper left corner ($T_{00} = 1$) gives exactly the definition of the 3×3 Z-matrix (2.82).

3. Convex Optimization

The numerical methods used in the publications of this thesis, can be formulated in three standard forms. The first is called linear programming in which the objective function which should be minimized as well as the constraints on the variables are all formulated as linear equations. The second method is called quadratic programming in which the constraints are still linear, but the objective function is a quadratic function of the variables. The third is called semi-definite programming where the variables are not vectors but positive-semi-definite matrices, and the objective function is a linear function of these matrices.

All three of these problems can be solved very efficiently with standard numerical methods. They are so effective that one can argue that formulating a problem in this form constitutes a solution of it. In the following we will give a brief summary of one solution method for linear programming, which is the easiest to understand. However, we will not describe the details of this method, but instead give an explicit example, which incorporates the general procedure, without taking into account all the special cases and complications, which might arise in general. For a more detailed description of the methods, we refer to Refs. [18, 19].

The definitions of the quadratic and semi-definite programs are given in the following and we refer to the Refs. [20, 21] for a description of the numerical solution methods.

3.1. Linear Programming

3.1.1. Standard form

A linear problem is an optimization task in which the objective function and the set of constraints are linear functions of the real variables. Every optimization problem of this type can be written in the standard form (SF), defined as

$$\min_{\mathbf{x}} \mathbf{c}^T \mathbf{x}, \quad \text{s.t.} \quad A\mathbf{x} = \mathbf{b}, \mathbf{x} \geq 0, \quad (3.1)$$

with A a real, not necessary square matrix and \mathbf{c} and \mathbf{b} real vectors. Additionally, all entries of the vector \mathbf{b} should be positive. The vector inequality $\mathbf{x} \geq 0$ is understood that every entry of the vector is larger or equal to zero. The vectors that satisfy the constraints are called **feasible** and the value of the objective function $\mathbf{c}^T \mathbf{x}$ will be called the **cost** of \mathbf{x} .

Every linear program can be transformed into this SF by adding additional variables, called **slack variables**. If some, or all, of the constraints are not given as equalities, but instead as inequalities, slack variables are used to transform these inequalities into equalities i.e. if an equation is given as $(A\mathbf{x})_j \geq b_j$, one reformulates it by demanding that

$$(A\mathbf{x})_j - s = b_j \tag{3.2}$$

with the new slack variable $s \geq 0$. This is equivalent to the original inequality. If the inequality is given as $(A\mathbf{x})_j \leq b_j$ the slack variable simply has a plus sign. The equation (3.2) can then again be written in the form $A'\mathbf{x}' = \mathbf{b}$, but with A extended to more columns and the variables into $\mathbf{x}' = (\mathbf{x}^T, \mathbf{s}^T)^T$, where the vector of slack variables \mathbf{s} has the length of the number of inequalities of the original program. To fulfill the condition that all entries of the vector \mathbf{b} should be positive, one can simply pick the negative entries $b_i < 0$ and multiply the equation $(A\mathbf{x})_i = b_i$ by -1 to get a new vector with all $b_i \geq 0$.

The slack variables can also be used to transform an unconstrained variable $x_j \in \mathbb{R}$ into

$$x_j = s_1 - s_2 \tag{3.3}$$

with $s_1, s_2 \geq 0$. In this way the variable is represented equivalently by two constraint variables. Another adjustment can be made if a variable is restricted to a subset of the real numbers: If a variable is restricted to $x_i \geq k$ this would give a new variable $y_i = x_i - k \geq 0$ with the b_j shifted to be $b_j - kA_{ji}$. And finally if the problem in question is a maximization problem the vector \mathbf{c} is replaced by $-\mathbf{c}$ to get the SF.

With those reformulations all linear programs can be written, without restriction of generality, in the standard form. Therefore, from here on, we will only consider programs of the type (3.1).

Example

Consider this transformation of a maximization problem into the SF.

Maximization problem	Converted into standard form
maximize $2x_1 - x_2 + 5x_3$	minimize $-2x_1 + x_2 - 5x_3$
subject to $2x_1 - x_2 - x_3 \geq -1$	subject to $-2x_1 + x_2 + x_3 + s_1 = 1$
$x_1 + 3x_3 \leq 7$	$x_1 + 3x_3 + s_2 = 7$
$-x_1 + 2x_2 \leq -4$	$x_1 - 2x_2 - s_3 = 4$
$x_1, x_2, x_3 \geq 0$	$x_1, x_2, x_3, s_1, s_2, s_3 \geq 0$

3.1.2. Dual Problem

For every linear problem one can define a so called **dual problem**, which is given as

$$\max_{\mathbf{y}} \mathbf{b}^T \mathbf{y}, \quad \text{s.t.} \quad A^T \mathbf{y} \leq \mathbf{c}, \mathbf{y} \geq 0, \quad (3.4)$$

with $\mathbf{c}, \mathbf{b}, A$ the same as in (3.1) and the $A^T \mathbf{y} \leq \mathbf{c}$ is understood for each entry. The dual problem has a very useful property, which is that it can be used to determine if an optimal solution of (3.1) is found by bounding the linear problem from below. Because for any feasible vector \mathbf{x} of the SF and any vector \mathbf{y} which satisfies the constraints of the dual problem, it holds that

$$\mathbf{c}^T \mathbf{x} \geq \mathbf{b}^T \mathbf{y}. \quad (3.5)$$

This can be proven by injecting the constraints as

$$\mathbf{c}^T \mathbf{x} = \mathbf{x}^T \mathbf{c} \geq \mathbf{x}^T (A^T \mathbf{y}) = (A\mathbf{x})^T \mathbf{y} = \mathbf{b}^T \mathbf{y}. \quad (3.6)$$

This fact is called weak duality. Therefore, the dual problem bounds the standard problem from below, and likewise the standard problem gives an upper bound on the dual problem. With that one can give a maximal error on an intermediate result, when the optimal value of the cost function is not yet found. The dual problem is also useful in detecting infeasibility, since if the SF is unbounded from below the dual problem is infeasible, and vice-versa, if the dual problem is unbound from above the SF is infeasible.

If the SF and the dual problem are both feasible, the **strong duality** holds [21]. It

states that the optimal solutions \mathbf{x}^* and \mathbf{y}^* of both problems coincide, as

$$\mathbf{c}^T \mathbf{x}^* = \mathbf{b}^T \mathbf{y}^*. \quad (3.7)$$

That means that there is no gap between the optimal solutions, thus, solving one problem also solves the other one.

3.1.3. Simplex algorithm

In the following we will describe an efficient way to find an optimal solution to a linear problem. There are two main ingredients in this approach, the first is the fact that all local extremas are global ones, and the second that every optimal solution can be written in a special form called basic solutions. Therefore one can search in the finite set of basic solutions for a local minimum. This minimum is then automatically the global minimum.

First note that the set of feasible vectors, i.e. vectors that satisfy $A\mathbf{x} = \mathbf{b}$, is a convex set. This can be seen easily by taking two feasible vectors \mathbf{x} and \mathbf{y} , and calculating all vectors in between with $r \in [0, 1]$ as

$$A[r\mathbf{x} + (1 - r)\mathbf{y}] = rA\mathbf{x} + (1 - r)A\mathbf{y} = r\mathbf{b} + (1 - r)\mathbf{b} = \mathbf{b}, \quad (3.8)$$

which shows that this vector is feasible for all $r \in [0, 1]$. We can use this fact to prove the following Theorem:

Theorem 1 ([18]). *Every local minimum of a linear problem in standard form is a global minimum.*

Proof. Let \mathbf{x} be a feasible vector, which is a local minimum and \mathbf{y} a feasible vector which is the global minimum. Additionally assume that $\mathbf{c}^T \mathbf{y} < \mathbf{c}^T \mathbf{x}$, so that the local minimum is not a global one. Take the feasible vector $\mathbf{z} = \epsilon \mathbf{x} + (1 - \epsilon)\mathbf{y}$ with $\epsilon \in (0, 1)$. Then

$$\mathbf{c}^T \mathbf{z} = \epsilon \mathbf{c}^T \mathbf{x} + (1 - \epsilon)\mathbf{c}^T \mathbf{y} < \epsilon \mathbf{c}^T \mathbf{x} + (1 - \epsilon)\mathbf{c}^T \mathbf{x} = \mathbf{c}^T \mathbf{x}, \quad (3.9)$$

hence, the vector \mathbf{z} has a smaller value of the cost function $\forall \epsilon \in (0, 1)$, therefore \mathbf{x} cannot be a local minimum. This contradicts the assumptions and, hence, proves the theorem. \square

Now we will define a basic solution. In the SF (3.1) assume that $A \in \mathbb{R}^{m \times n}$, with $m < n$, $\text{rank}(A) = m$. This is always possible by introducing new variables that do not

enter in the cost function. Then we can rearrange the columns of A in such a way that the first m columns are linearly independent and appear first as entries of a non-singular square matrix B , such that $A = [B, D]$ with D an $m \times (n - m)$ matrix with the remaining columns of A . With that a solution for the system of equations

$$Ax = \mathbf{b} \tag{3.10}$$

is given as $\mathbf{x} = [\mathbf{x}_B^T, \mathbf{0}^T]^T$, with $\mathbf{0}$ the vector of zeros, and

$$\mathbf{x}_B = B^{-1}\mathbf{b}. \tag{3.11}$$

The solutions of the form $[\mathbf{x}_B^T, \mathbf{0}^T]^T$ are called basic solutions with respect to the basis B . The variables \mathbf{x}_B are called **basic variables** and the variables which were set to zero are **non-basic variables**.

However, they do not need to be feasible, i.e. some entries of x_B might be negative. But this is not a fundamental problem since the optimal solution to the optimization in SF can always be written as a basic feasible solution:

Theorem 2 (Fundamental Theorem of linear programming¹).

1. *If there exists a feasible solution, then there exists a basic feasible solution.*
2. *If there exists an optimal solution, then there exists an optimal basic feasible solution.*

Therefore it is enough to search for an optimal solution in the finite subset of feasible basic solutions. One can cycle through the solutions in a systematic way such that the costs of each new step is at least as small as the previous one. If one reaches a step from which there is no improvement possible the solution is the desired optimal solution. This uses that every local minimum is immediately a global minimum, because of the convexity of the feasible set, as shown in Theorem 1. This method is called simplex algorithm and it can be schematically given as

1. Find an initial basic feasible solution as starting point. Go to Step 2.
2. Check if the basic feasible solution is optimal or if the linear problem is unbounded. If so Stop, if not go to Step 3.

¹The proof of this theorem can be found in [21].

3. Generate another basic feasible solution with a smaller value of the cost function and go to Step 2.

The step 3 of the algorithm is essentially exchanging the role of a basis variable with a non-basis variable, in such a way that the new cost function has a smaller value for its basic solution. There exists heuristics that make sure to exchange the two variables with the biggest influence on the value of the cost function first, and also methods to avoid to be stuck in a circle, i.e. to reach a basic solution already considered. We will not give the details of the various implementations, such as how to find the basic feasible solution in Step 1 in general. The interested reader is referred to the books [21, 18] for the details. Instead we will present an example of the simplex method which exemplifies the main ideas.

Example of the simplex algorithm

Consider this linear problem in standard form:

$$\text{minimize } x_1 - 2x_2 - 3x_3 \tag{3.12}$$

$$\text{subject to } 2x_1 - x_2 - x_3 + 11 = s_1 \tag{3.13}$$

$$-x_1 - 3x_3 + 3 = s_2 \tag{3.14}$$

$$x_1 - 2x_2 + 8 = s_3 \tag{3.15}$$

$$x_1, x_2, x_3, s_1, s_2, s_3 \geq 0. \tag{3.16}$$

A feasible basic solution can be read of as $(x_1, x_2, x_3, s_1, s_2, s_3)^T = (0, 0, 0, 11, 3, 8)^T$, therefore s_1, s_2, s_3 are the basic variables. The cost of this feasible basic solution is 0. It is however not optimal since there are negative coefficients of x_2 and x_3 . Therefore one can lower the cost by increasing these two variables. As a next step we will exchange a non-basic variable with a basic one. We pick x_3 since it has the strongest influence on the costs. The variable x_3 is restricted by the first two constraints (with keeping $x_1 = x_2 = 0$), to $x_3 \leq 11$ and $x_3 \leq 1$. Where the values of s_1 and s_2 are assumed to be larger or equal to zero, but not anymore fixed to the values given in the basic feasible solution.

Note that if the constraints would not give an upper bound on x_3 the linear problem would be unbounded, since then the variable could be made arbitrary large, without

violating the constraints, and therefore the costs of this vector could reach $-\infty$.

However, since the variable is bounded, we can continue by picking the second constraint for the exchange since it gives a stronger restriction to the variable. So we switch the role of x_3 with s_2 . Rearranging (3.14) gives

$$-\frac{1}{3}x_1 - \frac{1}{3}s_2 + 1 = x_3 \quad (3.17)$$

and thus the equivalent linear problem reads,

$$\text{minimize } 2x_1 - 2x_2 + s_2 - 3 \quad (3.18)$$

$$\text{subject to } \frac{7}{3}x_1 - x_2 + \frac{1}{3}s_2 + 10 = s_1 \quad (3.19)$$

$$-\frac{1}{3}x_1 - \frac{1}{3}s_2 + 1 = x_3 \quad (3.20)$$

$$x_1 - 2x_2 + 8 = s_3 \quad (3.21)$$

$$x_1, x_2, x_3, s_1, s_2, s_3 \geq 0. \quad (3.22)$$

Now we get the basic solution as $(x_1, x_2, x_3, s_1, s_2, s_3)^T = (0, 0, 1, 10, 0, 8)^T$ with a value of the cost function -3 , this basic feasible solution is also not optimal, since the coefficient of x_2 is still negative. So we exchange x_2 with one of the basic variables s_1 or s_3 . The restriction from the variable s_1 is $x_2 \leq 10$, but the restriction from s_3 is stronger as it gives $x_2 \leq 4$. Therefore we exchange x_2 with s_3 . Rearranging Eq. (3.21) gives then

$$\frac{1}{2}x_1 - \frac{1}{2}s_3 + 4 = x_2 \quad (3.23)$$

and the new linear problem is

$$\text{minimize } x_1 + s_2 + s_3 - 11 \quad (3.24)$$

$$\text{subject to } \frac{11}{6}x_1 + \frac{1}{3}s_2 + \frac{1}{2}s_3 + 6 = s_1 \quad (3.25)$$

$$-\frac{1}{3}x_1 - \frac{1}{3}s_2 + 1 = x_3 \quad (3.26)$$

$$\frac{1}{2}x_1 - \frac{1}{2}s_3 + 4 = x_2 \quad (3.27)$$

$$x_1, x_2, x_3, s_1, s_2, s_3 \geq 0. \quad (3.28)$$

The basic feasible solution of this is $(x_1, x_2, x_3, s_1, s_2, s_3)^T = (0, 4, 1, 6, 0, 0)^T$, with the value of the cost function -11 . This solution is a local minimum, because all variables

have positive coefficients, so changing x_1, s_2 or s_3 to a value larger than zero can only increase the costs. Using Theorem 1, we conclude that we have found the global minimum of the given problem (3.12).

3.2. Quadratic Programming

A quadratic optimization problem with linear constraints is of the form

$$\min_{\mathbf{x}} \frac{1}{2} \mathbf{x}^T Q \mathbf{x} + \mathbf{c}^T \mathbf{x} \quad \text{s.t.} \quad A \mathbf{x} \leq \mathbf{b}, \mathbf{x} \geq 0, \quad (3.29)$$

with A a real matrix, \mathbf{c} and \mathbf{b} real vectors and Q a real square matrix. The equation $A \mathbf{x} \leq \mathbf{b}$ and the inequality $\mathbf{x} \geq 0$ are understood for each component of the vector.

One special case of these problems arise if the matrix Q is positive semi-definite. In this case a set of necessary conditions for optimality, i.e. that a point x^* is the global minimum of the problem, becomes a set of necessary and sufficient conditions. These are called the Karush-Kuhn-Tucker conditions [22] and they can be derived [23] from the Lagrange function

$$L(\mathbf{x}, \boldsymbol{\mu}) = \mathbf{c}^T \mathbf{x} + \frac{1}{2} \mathbf{x}^T Q \mathbf{x} + \boldsymbol{\mu} (A \mathbf{x} - \mathbf{b}) \quad (3.30)$$

with $\boldsymbol{\mu}$ the row-vector of Lagrange multipliers, to be

$$\frac{\partial L}{\partial x_j} \geq 0, \quad \frac{\partial L}{\partial \mu_i} \leq 0, \quad x_j \frac{\partial L}{\partial x_j} = 0, \quad \mu_i (A \mathbf{x} - \mathbf{b})_i = 0, \quad x_j \geq 0, \quad \mu_i \geq 0, \quad \forall i, j. \quad (3.31)$$

By introducing two vectors of slack variables $\mathbf{y} \geq 0$ and $\mathbf{v} \geq 0$ the conditions (3.31) can be written in a more compact form as,

$$Q \mathbf{x} + A^T \boldsymbol{\mu}^T - \mathbf{y} = -\mathbf{c}^T, \quad (3.32)$$

$$A \mathbf{x} + \mathbf{v} = \mathbf{b}, \quad (3.33)$$

$$\mathbf{x} \geq 0, \boldsymbol{\mu} \geq 0, \mathbf{y} \geq 0, \mathbf{v} \geq 0, \quad (3.34)$$

$$\mathbf{y}^T \mathbf{x} = 0, \boldsymbol{\mu} \mathbf{v} = 0. \quad (3.35)$$

Note that the first two lines are just linear equalities. So a global minimum of the quadratic problem can be found by searching for a point that satisfies the conditions (3.32)-(3.35). This can be achieved e.g. with an adjusted simplex algorithm [23] or by

employing the Cholesky decomposition to get a Newton step [24] in the direction of a solution (for details see [25]).

3.3. Semi-definite Programming

A semi-definite problem [26] can be written as

$$\min_{\mathbf{x}} \mathbf{c}^T \mathbf{x}, \quad \text{s.t.} \quad F(\mathbf{x}) \geq 0, \quad (3.36)$$

$$F(\mathbf{x}) = F_0 + \sum_{i=1}^m x_i F_i, \quad (3.37)$$

with the minimization over a vector of real variables \mathbf{x} . The F_i are real symmetric matrices, and the inequality sign in $F(\mathbf{x}) \geq 0$ means that the matrix $F(\mathbf{x})$ is positive semi-definite. These types of problems are more general than the linear and quadratic problems given in Sections 3.1 and 3.2, because one can always write a linear or quadratic problem in the form of a semi-definite problem (3.36) by choosing the matrices F_i and the vector \mathbf{c} accordingly. However, from a computational point this would not be efficient, since the more specialized numerical solution methods for linear and quadratic problems are, in general, faster.

Nevertheless these semi-definite problems are not much harder to solve than the linear or quadratic problems. This is due to the fact that these problems are convex, i.e. if $F(\mathbf{x}) \geq 0$ and $F(\mathbf{y}) \geq 0$ then

$$F(\lambda \mathbf{x} + (1 - \lambda) \mathbf{y}) = \lambda F(\mathbf{x}) + (1 - \lambda) F(\mathbf{y}) \geq 0 \quad (3.38)$$

for $\lambda \in [0, 1]$. With this it follows that a local minimum is also the global one, by the same reasoning as in Theorem 1 on page 27.

By using the property of convexity the semi-definite problems can be solved e.g. with primal-dual interior point methods [27, 28, 26], where these methods are generalizations of interior point methods originally derived for linear problems.

4. Results and Outlook

4.1. Framework

The main topic of this thesis is the study of entanglement of multi-partite states. This genuine quantum feature is the cornerstone of many applications and possible future technologies, such as quantum computation [29, 30], quantum cryptography [31] or quantum metrology¹ [33]. It is also conceptually fascinating, since one can argue that it embodies the core essence of quantum theory, or as Schrödinger put it [34],

I would not call that *one* but rather *the* characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought.

In our research we focused mainly on symmetric quantum states, i.e. pure states invariant under permutation of particles and mixtures of such states. This has the main advantage that the Hilbert space used to describe these states only grows linearly with the number of constituents, in contrast to the exponential growth of the full Hilbert space of multi-partite systems with the number of particles. This restriction makes even large number of particles experimentally [35] and computationally accessible. But symmetric states have other useful properties besides being more tractable. It was for example shown that random symmetric states, in general, achieve Heisenberg scaling in quantum enhanced measurements, while random non-symmetric states, even after local unitary optimization, do not [36].

The close investigation of symmetric states can also be helpful in deriving results for a more general class of states, i.e. it was possible to derive a numerical method that detects entanglement or separability in quantum states of arbitrary, finite, size for any partition into sub-systems desired.

¹Although there exist quantum enhanced measurements schemes that do not require entanglement [32].

4.1.1. Partial transpose criteria for symmetric states

The tensor representation of spin- j states [6] was a central tool and starting point for the derivation of many of the results presented in this thesis. This tensor representation is a generalization of the familiar Bloch-vector representation of spin-1/2 states to spin- j states, with $j > \frac{1}{2}$. This tensor representation of a spin- j state ρ is given as,

$$X_{\mu_1 \dots \mu_N} = \text{tr} \left\{ \rho P_s (\sigma_{\mu_1} \otimes \dots \otimes \sigma_{\mu_N}) P_s^\dagger \right\}, \quad (4.1)$$

with P_s the projector onto the symmetric subspace of tensor products of spins-1/2, $N = 2j$, σ_0 the 2×2 identity matrix, and σ_k , $k \in \{1, 2, 3\}$ the usual Pauli matrices. As we have seen in section 2.3.1, a spin- j state is equivalent to a symmetric state of N qubits. Hence, the tensor representation X can also be seen as a representation of the latter.

Using this tensor it is possible to find a simple way to write down the partial transpose criterion as condition on the real matrix

$$T_{\boldsymbol{\mu}, \boldsymbol{\nu}} = X_{\mu_1 \dots \mu_j \nu_1 \dots \nu_j}, \quad (4.2)$$

where the matrix indices are vectors, with $\boldsymbol{\mu} = (\mu_1 \dots \mu_j)$ and $\boldsymbol{\nu} = (\nu_1 \dots \nu_j)$. The partial transpose criterion for the state ρ is then equivalent to the condition

$$T_{\boldsymbol{\mu}, \boldsymbol{\nu}} \geq 0, \quad (4.3)$$

because this matrix is similar (i.e. it has the same eigenvalues) up to a factor, to the density matrix of the partial transposed state.

This identification allowed us to show that some separability or classicity criteria are equivalent to the partial transpose criterion. For example, the Z -matrix [11] of a spin-1 state is similar to the partial transposed state of a symmetric state of two qubits. Positivity of the correlation matrix in [37] was already proven to be equivalent to the partial transpose criterion, however, showing that this matrix is just the Schur complement of the matrix T , gives a more direct proof of this fact.

The same connection also holds for the correlation matrices of local observables as given in [38]: They too are Schur complements of the matrix T . But most striking, a reduced version of the matrix T plays also a central role in Lasserre's method of polynomial optimization [39] under the name moment matrix. This showed that there is a deep connection between the entanglement problem in physics and the mathematical fields of

polynomial optimization as well as the problem of truncated moment sequences, i.e. the question if a certain set of moment values is compatible with a positive measure.

4.1.2. Truncated moment sequences for entanglement detection

In fact, the entanglement problem, i.e. the question if a state is entangled or separable, can be mapped onto a truncated moment problem. With that mapping we could use numerical tools designed for the truncated moment problem to decide if a state is separable or not. This is done by a semi-definite program which gives an answer to this question in a finite number of steps, and if a state is separable it also gives an explicit decomposition into separable states with almost no extra costs. If this numerical method is applied to symmetric states, the simpler structure of those states can be easily accounted for and it results in a large computational speed-up.

This numerical algorithm is an extension of the known methods of semi-definite programming for the entanglement problem [40, 41, 42, 43], in which extensions of a state were constructed to detect entanglement. Our approach unifies some of these methods in a more abstract way and fills some interpretational gaps of the semi-definite algorithms, e.g. the central role of the moment matrix as representation of the partial transpose criterion. By using the software GloptiPoly 3 [44] it was possible to give a very short implementation of this method in the software MATLAB.

This method can also be used for other tasks, e.g. to numerically investigate the minimal number of pure separable symmetric states necessary to construct every mixed separable symmetric state, or to test if the marginals, i.e. states after partial tracing, are sufficient to detect entanglement in the original state, even when the marginals are, themselves, all separable [45].

From an experimental point of view it is desirable to conclude from a partial set of measurement results that a state had to be entangled. This question can be directly addressed with the formulation as truncated moment problem, by just not fixing the unknown measurement results in the definition of the truncated moment problem.

4.1.3. Numerical tools to compute quantumness

The numerical method for the truncated moment problem gives a certificate of entanglement, but it does not give information on the amount of entanglement. For this task we improved existing numerical methods to determine the Hilbert-Schmidt distance of a symmetric multi-qubit state to the convex hull of separable symmetric states, defined

by the term "quantumness" [46], given as

$$Q(\rho) = \min_{\rho_c \in \mathcal{C}} \|\rho - \rho_c\|, \quad (4.4)$$

with \mathcal{C} denoting all separable symmetric states.

To determine this minimum, we developed a two step algorithm, where the main ingredient is not to optimize over the full set of separable symmetric states, but instead only over a computationally manageable approximation of it. This approximation are all states that can be constructed by mixing a large number of pre-chosen fixed separable states $\{\phi_i\}$, as

$$Q(\rho) \leq \min_{w_i, \sum_i w_i=1} \|\rho - \sum_i w_i |\phi_i\rangle \langle \phi_i|\|. \quad (4.5)$$

This gives an upper bound, because the optimization on the right-hand-side is performed just over a sub-set of all separable symmetric states \mathcal{C} . This bound can be calculated efficiently since the right-hand-side of (4.5) can be transformed into a quadratic optimization program in the real variables w_i . For computational reasons, we also split the set $\{\phi_i\}$ into smaller sub-sets and optimize over them one by one. To mitigate the negative effects of this splitting, we add the states which had the largest weights in the previous iteration to the next subset of pre-chosen states. When the quadratic program terminates it gives an approximation of the closest symmetric separable state $\tilde{\sigma}$, and hence an upper bound on the quantumness (4.4).

This approximated closest separable state is the starting point in refining the approximation by moving the state $\tilde{\sigma}$ as far as possible into the direction of ρ , under the constraint that it stays separable. Again we just approximate the separable states by a mixture of a finite sample $\{\phi_i\}$ of pre-chosen separable states. This can be formulated as a linear optimization task as,

$$\max_{k, w_i} k, \quad \text{s.t.} \quad k\rho + (1-k)\tilde{\sigma} = \sum_i w_i |\phi_i\rangle \langle \phi_i|, \quad (4.6)$$

where $k \in [0, 1]$ parametrizes the line between ρ and $\tilde{\sigma}$.

This second step usually slightly improves the approximation of the quadratic optimization (4.5), because the number of states $\{\phi_i\}$ used, can be much larger, e.g. two orders of magnitude, due to the faster execution time of a linear optimization problem. This decreases the upper bound usually by a value smaller than 10^{-4} .

This gain in accuracy to the methods used before [46], was the starting point in the successful search for an analytic solution to the aforementioned problem in the case of symmetric two-qubit pure states.

4.1.4. Quantumness of spin-1

We found an explicit analytic formula for the closest separable symmetric state of an arbitrary symmetric pure state, and hence a direct formula for the minimal Hilbert-Schmidt distance to the set of symmetric separable states.

Interestingly, the distance depends only on a single parameter, the smallest eigenvalue λ_{\min} of the matrix T (4.2). As we have mentioned earlier the matrix T is similar to the partial transposed density matrix by a simple factor, hence, λ_{\min} is equal to twice the negativity of the state, i.e. the smallest eigenvalue of the partial transpose states. It is well known, that for two qubits, $\lambda_{\min} < 0$ is a necessary and sufficient entanglement criterion. But now λ_{\min} is also the parameter of a geometric property of entanglement, i.e. the minimal distance to the separable symmetric states. This analytic formula is found to be,

$$Q(|\psi\rangle) = f(\lambda_{\min}) = \begin{cases} -\sqrt{\frac{3}{8}}\lambda_{\min} & \text{for } \lambda_{\min} \leq -\frac{1}{2}, \\ h(\lambda_{\min}) & \text{for } \lambda_{\min} > -\frac{1}{2}. \end{cases} \quad (4.7)$$

It is linear in λ_{\min} , for highly entangled states, but for weaker entangled states ($\lambda_{\min} > -1/2$) its expression is quite complicated, however, $h(\lambda_{\min})$ can still be given as a closed expression. The formula (4.7) was derived by finding the explicit form of the closest separable symmetric state for any pure state. These states are all mixed states, except in the case when the pure state is itself separable and, hence, it is its own closed separable state.

The case of mixed states is more complex in the sense that the distance seems not to depend anymore on a single parameter. However, we conjectured that the pure state result serves as upper bound of the quantumness of a general mixed symmetric state of two qubits. Unfortunately, we were not able to prove this in the general case, but just for special sub-classes of mixed states, namely all states on a line between a pure state and its closest classical state. Nonetheless, we have strong numerical evidence that the conjectured upper bound

$$Q(\rho) \leq f(\lambda_{\min}) \quad (4.8)$$

is in fact true. This was shown with the two step quadratic-linear program, which gives upper bounds on the quantumness of a given state. In every random state tested, it was possible to decrease the approximated quantumness below the upper bound given by $f(\lambda_{\min})$, where λ_{\min} is also the smallest eigenvalue of the matrix T of the states. This indicates that λ_{\min} is the best choice to parameterize the distance to the set of symmetric separable states.

Additionally, we were able to prove a lower bound on the quantumness of mixed states, as

$$Q(\rho) \geq -\frac{\lambda_{\min}}{\sqrt{3}}. \quad (4.9)$$

This lower bound was found by optimizing, not as in Eq. (4.5) over a smaller set than all separable states, but instead of lifting some requirements that the matrix ρ_c represents a valid symmetric multi-qubit state. Then, a careful reparameterization allowed to simplify the minimization task into a form that could be solved analytically.

4.1.5. Absolutely classical states

Since, separable symmetric multi-qubit pure states can be identified with spin coherent states, this equivalence allows one to write the definition of separability as a condition on the P-function, as given in Eq. (2.72): A state is separable (or classical) if, and only if, there exists a $P(\alpha) \geq 0$ that represents this state. We utilized this definition to investigate the set of absolutely classical states, which are states that remain classical, i.e. separable, under any unitary transformation.

The maximally mixed symmetric state is an absolutely classical state. Therefore we asked the question what is the largest distance around the maximally mixed state, in which all states are absolutely classical. We were able to find a lower bound on the largest ball radius of absolutely classical states around the maximally mixed state for any system size. This bound is found to be

$$\left\{ (1 + N) \left[(4N + 2) \binom{2N}{N} - (N + 2) \right] \right\}^{-1/2} \leq B_N, \quad (4.10)$$

for symmetric states of N qubits, so that all states that fulfill

$$\|\rho - \rho_0\| \leq B_N, \quad (4.11)$$

are separable and stays separable under any (possible non-local) unitary transformation, with ρ_0 the maximally mixed state of the symmetric subspace of N -qubits, and the distance measured with the Hilbert-Schmidt norm. This bound was found by expanding the P-function over the spherical harmonics and then using the Cauchy-Schwarz inequality to get a condition on the positivity of the P-function.

To test the sharpness of the bound (4.10), we conducted a numerical search by linear programming to get an upper bound on the maximal radius of absolutely classical states, by searching for a non-classical state as close as possible to the maximally mixed state. These bounds are schematically depicted in Fig. 4.1, where the outer circle depicts the numerically found upper bound and the inner circle the bound given by Eq. (4.10).

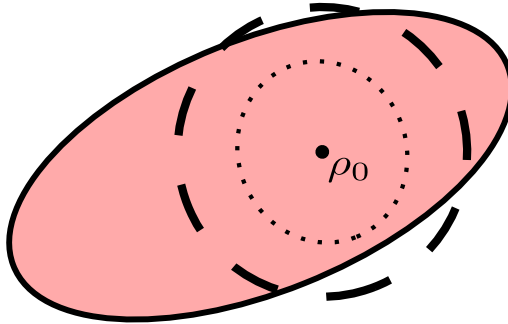


Figure 4.1.: A visualization of the absolute separable states marked as light red area. The lower bound (4.10) is marked as dotted circle around the maximally mixed symmetric state ρ_0 . The upper bound is marked as the dashed circle. This upper bound was found by searching for an entangled state as close as possible to the maximally mixed symmetric state. The scaling of this figure does not correspond to the real values. It should be noted that there are absolutely classical states further away than the upper bound of the largest ball of absolutely classical states, which corresponds to the colored area at a larger distance than the outer circle.

A similar question was already investigated in the case of non-symmetric states in [47]. The restriction onto symmetric states changes the problem, since the set of allowed states is smaller, which makes the problem more challenging. Also the maximally mixed states of the symmetric states and of the full states are centered at different positions, therefore we did not expect that the results would give comparable values. Surprisingly the numerical values were nonetheless comparable to the non-symmetric case, however, we know that they cannot be the same. This can be deduced from the case of the symmetric states of two qubits, since there, the full analytic parameterization of the separable states is known [48]. Hence, in this case, the largest separable ball can be calculated analytically and the symmetric and non-symmetric results do not coincide,

thus showing that the largest separable balls have different sizes.

4.1.6. Tensor eigenvalues for entanglement detection

The identification of a symmetric multi-qubit state with a tensor allowed to make another interesting finding, which relates the spectral properties of a tensor to the entanglement problem.

The definition of positive semi-definiteness of a tensor coincides with a necessary condition for separability of a symmetric state of an even number N of qubits. Therefore if the tensor representation $X_{\mu_1 \dots \mu_N}$ of a state ρ is not positive semi-definite the state is entangled. A way to determine if a tensor is positive semi-definite is to calculate the tensor eigenvalues. These are generalizations of the usual matrix eigenvalues, however, they are more complicated to calculate, since it involves non-linear optimizations and there are different definitions of tensor eigenvalues in the literature [49].

We choose a type of tensor eigenvalues called 'Z-eigenvalues' [50], which is invariant under rotations and which has the property that a tensor is positive semi-definite if and only if the smallest tensor eigenvalue λ_{\min} is non-negative. That allowed us to link the value of the smallest tensor eigenvalue to the entanglement properties of a quantum state: If $\lambda_{\min} < 0$ the state is entangled.

This criterion works well for highly entangled states, however, very weakly entangled states are not reliably detected. This is not a contradiction, since it is only a necessary condition for entanglement and weakly entangled states can have a positive semi-definite tensor representation.

Inspired by the entanglement measure 'negativity' [51], we investigated if and how the magnitude of the smallest tensor eigenvalue is correlated to the amount of entanglement, measured as the Hilbert-Schmidt distance to the convex hull of separable symmetric states. For small system sizes, i.e. $N \leq 6$ there is a strong correlation, however, this correlation gets weaker with increasing system size. In the case of twelve qubits the correlation between the value of the smallest tensor eigenvalue and the quantumness is almost gone. This means that a state with e.g. $\lambda_{\min} = -0.5$ is not necessarily more entangled than a state with $\lambda_{\min} = -0.2$.

4.1.7. Tensor classes for separable states

The connection between the spectral properties of a tensor with the entanglement problem of symmetric states, inspired the definition of a new type of tensors called the

regularly decomposable tensors. This mathematical formulation of the quantum entanglement problem allowed us to clearly define separability in the formal mathematical language of tensor theory, and to generalize the description, so that also half-integer values of j , i.e. an odd number of qubits, can be investigated. With that, it was shown that a tensor, which represents a symmetric state of qubits, is a regularly decomposable tensor if and only if the state is separable.

4.2. Future endeavors

4.2.1. Efficient partial transpose implementations

The size of the Hilbert space of a symmetric multi-qubit state scales only linearly with the number of qubits. However, a direct implementation of the partial transpose criterion embeds the state in the exponentially large Hilbert space of N qubits, and therefore requires to compute the positive definiteness of a matrix of size $2^N \times 2^N$. The matrix T , which is similar, up to a factor, to the partial transposed density matrix of bipartition into equally sized parts, can be reduced in size by removing recurring rows and columns, which does not change the positive-semi-definiteness of T . In this way the partial transpose criterion between two equally sized partitions can be implemented as a condition on a square matrix with number of rows equal to $\frac{1}{6}(N+2)(N+3)(N+4)$. This connection should be extendable to the case of an uneven number of qubits, and of different numbers of transposed qubits, and not just to a partition into equally sized subsystems.

This question was already investigated in [52], where the partial transpose criterion was implemented on a matrix whose size scales quadratically in the number of qubits. It would be interesting to see, how the reduced version of the matrix T relates to these results.

4.2.2. Polynomial optimization in relation to the entanglement problem

There is still all lot of work to be done in working out the details between the entanglement problem and the connection with polynomial optimization. For example, it would be interesting to investigate the connection between positive polynomials, which are not sum-of-square polynomials, with the concept of bound entangled states, i.e. entangled

states which have a positive partial transpose. This question is related to Hilbert's 17th problem [53] and was already investigated in [54, 55].

It would be also interesting to apply the physical interpretation of the concept of partial transposition on the purely mathematical field of polynomial optimization, to get a better intuition on the methods employed there. This showed to be a fruitful direction already, by translating the well known fact that the partial transpose criterion is necessary and sufficient for a qubit-qutrit system, into the language of truncated moment sequences. This gave a solution to a particular subclass of moment problems, and this solution seemed to be unknown in the mathematical community.

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5. Contributions to the Publications



Erklärung nach § 5 Abs. 2 Nr. 8 der Promotionsordnung der Math.-Nat. Fakultät
-Anteil an gemeinschaftlichen Veröffentlichungen-
Nur bei kumulativer Dissertation erforderlich!

Declaration according to § 5 Abs. 2 No. 8 of the PromO of the Faculty of Science
-Share in publications done in team work-

Name: Fabian Bohnet-Waldruff

List of Publications

1. F. Bohnet-Waldruff, D. Braun, and O. Giraud, Physical Review A **93**, 012104 (2016).
2. F. Bohnet-Waldruff, D. Braun, and O. Giraud, Physical Review A **94**, 042343 (2016).
3. F. Bohnet-Waldruff, D. Braun, and O. Giraud, Physical Review A **94**, 042324 (2016).
4. F. Bohnet-Waldruff, O. Giraud, and D. Braun, Physical Review A **95**, 012318 (2017).
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6. F. Bohnet-Waldruff, D. Braun, and O. Giraud, arXiv:1704.02277v1 [quant-ph] (2017).
Submitted to Physical Review A.

Nr.	Accepted for publication yes/no	Number of all authors	Position of the candidate in list of authors	Scientific ideas of candidate (%)	Data generation by candidate (%)	Analysis and Interpretation by candidate (%)	Paper writing by candidate (%)
1	Yes	3	First	80	100	80	80
2	Yes	3	First	20	No data	33	20
3	Yes	3	First	70	100	80	70
4	Yes	3	First	33	100	50	40
5	Yes	5	Fourth	10	No data	5	5
6	No	3	First	50	100	70	50

I certify that the above statement is correct.

Date, Signature of the candidate

I/We certify that the above statement is correct.

Date, Signature of the doctoral committee or at least of one of the supervisors

A. Publications

A.1. Quantumness of spin-1 states

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Quantumness of spin-1 states

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We investigate quantumness of spin-1 states, defined as the Hilbert-Schmidt distance to the convex hull of spin coherent states. We derive its analytic expression in the case of pure states as a function of the smallest eigenvalue of the Bloch matrix and give explicitly the closest classical state for an arbitrary pure state. Numerical evidence is given that the exact formula for pure states provides an upper bound on the quantumness of mixed states. Due to the connection between quantumness and entanglement we obtain new insights into the geometry of symmetric entangled states.

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I. INTRODUCTION

The quantum world is the realm of the most counterintuitive phenomena, from the tunnel effect to the more recent quantum teleportation. There are, however, instances of quantum states which behave in an almost classical way. The best-known example of such a behavior is that of coherent states. With the rise of quantum information technology the need to identify genuine quantum states, where truly quantum phenomena could occur, has become important. Several notions of “quantumness” exist, emphasizing different physical consequences of quantum behavior. One of the oldest ones goes back to quantum optics, where coherent states of light are considered the most classical pure states possible. These are states with minimal quantum uncertainty in the quadratures, i.e., localized as much as possible in phase space, and this property is preserved under the free time evolution of the electromagnetic field [1]. The purely classical procedure of randomly choosing such states adds classical noise but no quantum noise. The resulting mixed states, whose Glauber representation is a convex combination of coherent state projectors, form a convex set of states with positive P function, and there is widespread agreement that such states are to be considered the most classical states [2,3]. Coherent states can be defined in other physical systems; see [4,5].

The definition of classicality was extended to finite-dimensional systems in [6], where spin-coherent states [SU(2) coherent states] play the role of the pure states with minimal quantum fluctuations of the angular-momentum operators [7]. The property of minimal quantum fluctuations is conserved under unitary operations representing rotations. A mixed state can be considered classical if it can be written as a statistical mixture of spin-coherent states, meaning that a representation with a positive P -function exists. The set of “classical spin states” can thus be defined as the convex hull of spin-coherent states [6,8]. Any state outside this set may be considered truly quantum. To measure the departure from the classical behavior it is convenient to define “quantumness” as the Hilbert-Schmidt distance from the state to the set of classical states [8,9]. Other quantifiers of quantumness are based on different sets of “classical states,” e.g., states with positive Wigner function [10], and use various measures of distance, such as the trace distance [11] or the Bures distance [12]. Note that different distance measures may lead to different ordering

of quantum states [13], a problem that was addressed by using a topological measure [14].

Alternative measures of quantumness are based on entanglement [15–17]. Even though formal analogies of entanglement can be found also in classical physics, and have attracted attention recently in optics [18], entanglement is a signature of a quantum behavior. Entangled quantum states can lead to stronger-than-classical correlations between subsystems. A number of entanglement measures have been proposed in order to quantify entanglement. A way of defining such a measure, in the case of finite-dimensional systems we consider here, is through the distance between a state and the convex set of separable states. While this distance was shown to yield a good measure of entanglement when it is taken as the relative entropy or the Bures distance [19,20], it is currently still unclear whether the Hilbert-Schmidt distance yields a good measure of entanglement [21], as it is not contractive [22]. However, this measure is mathematically convenient as a Euclidean distance on Hilbert space, and has nice physical properties. For instance, the Hilbert-Schmidt distance is equal to the maximum amount by which a certain type of a generalized Bell inequality is violated [23]. Furthermore, we show here that the Hilbert-Schmidt distance gives new insight into the geometry of entangled states.

In the present paper, we investigate the problem of finding the distance from a state to the set of classical states, as well as the classical state closest to a given state. The closely related problem of finding the *separable* state closest to a given state has already been investigated in the literature. For instance, if one restricts the set of separable states to pure states then it was shown in [24] that the closest separable pure state in terms of Bures distance to a pure symmetric state is always symmetric. This result also holds for the Hilbert-Schmidt distance as both distances are simply related to the overlap of the two states in this pure state case. In [25], the problem of the Hilbert-Schmidt distance from a bipartite two-qubit state to the closest (possibly mixed) separable state was investigated. Specializing the results of [25] to symmetric states, one can observe that the separable state closest to a symmetric state (pure or not) is in general mixed and not necessarily symmetric.

Here we solve the problem of finding the classical state closest to a general spin-1 state, in terms of the Hilbert-Schmidt distance. We find an analytical solution for pure states. Our findings generalize a result obtained in [9] for the most

quantum spin-1 pure state. As we will see, this also solves the problem of finding the symmetric separable state closest to a pure symmetric bipartite state of two qubits.

The paper is organized as follows. In Sec. II we introduce the Bloch matrix representation that we will use throughout the paper. Section III solves the problem of finding the classical state closest to any given pure spin-1 state, while Sec. IV tackles the problem for mixed states. Section V makes the connection with entanglement and entanglement measures.

II. DEFINITIONS

A. Tensor representation

A way of representing spin- j states which is particularly convenient when dealing with spin-coherent states is the tensor representation proposed in [26]. It is a generalization of the well-known Bloch picture for spin- $\frac{1}{2}$ states. In the case $j = \frac{1}{2}$, any state ρ can be expanded as

$$\rho = \frac{1}{2} \sum_{\mu=0}^3 X_{\mu} S_{\mu}, \quad (1)$$

with S_0 the 2×2 identity matrix, and $S_i = \sigma_i$, $1 \leq i \leq 3$, the three Pauli matrices. In this basis, the coordinates of ρ are $X_0 = 1$ and $X_i = \text{tr}(\rho S_i)$, so that $\mathbf{X} = (X_1, X_2, X_3)$ forms the usual Bloch vector.

For higher spin, it is possible to associate with any spin- j state ρ a tensor with $2j$ indices [26]. For spin-1 this tensor reduces to a matrix that can be defined as

$$X_{\mu\nu} = \text{tr}(\rho S_{\mu\nu}), \quad 0 \leq \mu, \nu \leq 3, \quad (2)$$

with $S_{00} = \mathbb{1}$, the 3×3 identity matrix, $S_{a0} = S_{0a} = J_a$, and $S_{ab} = J_a J_b + J_b J_a - \delta_{ab} \mathbb{1}$, where J_a is the usual spin-1 angular momentum operator, $1 \leq a, b \leq 3$ (here we take $\hbar = 1$). The matrices $S_{\mu\nu}$ are such that ρ can be expanded as

$$\rho = \frac{1}{4} \sum_{\mu, \nu=0}^3 X_{\mu\nu} S_{\mu\nu}. \quad (3)$$

The 4×4 matrix X is real and symmetric with trace two. As in the spin- $\frac{1}{2}$ case, where the Bloch vector transforms as a three-dimensional (3D) vector under rotations of the coordinate frame, for spin-1, X transforms under a 3D rotation according to $X' = R X R^\dagger$, with R_{ab} , $1 \leq a, b \leq 3$, the 3×3 rotation matrix, and $R_{0\mu} = R_{\mu 0} = \delta_{\mu 0}$, $0 \leq \mu \leq 3$. We will thus call X the Bloch matrix.

This representation is particularly well-suited to our problem, since, as we will see, coherent states take a very simple form in this framework.

B. Quantumness

The set \mathcal{C} of classical spin states is defined [6] as the ensemble of all density matrices which can be expressed as a mixture of spin-coherent states with positive weights, i.e., states ρ_c for which there exist weights $w_i \geq 0$ and coherent states $|\alpha_i\rangle$ such that

$$\rho_c = \sum_i w_i |\alpha_i\rangle \langle \alpha_i|, \quad (4)$$

with $0 \leq w_i \leq 1$, and $\sum_i w_i = 1$. Here we use the following definition of spin-coherent states $|\alpha\rangle = |\theta, \phi\rangle$, with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi[$ the usual spherical angles,

$$|\alpha\rangle = \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2} e^{-i\phi}\right)^{j-m} |j, m\rangle, \quad (5)$$

where $|j, m\rangle$ is the usual spin basis, here with $j = 1$ and $m = -1, 0, 1$.

The Bloch matrix of a coherent state takes the simple form $X_{\mu\nu} = n_{\mu} n_{\nu}$, $0 \leq \mu, \nu \leq 3$, with $n_0 = 1$ and $\mathbf{n} = (n_1, n_2, n_3) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. The decomposition (4) can be reexpressed in terms of the Bloch matrix W of ρ_c as

$$W_{\mu\nu} = \text{tr}(\rho_c S_{\mu\nu}) = \sum_i w_i n_{\mu}^{(i)} n_{\nu}^{(i)}, \quad (6)$$

with $\mathbf{n}^{(i)} = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i)$ the Bloch vectors corresponding to coherent states $|\alpha_i\rangle$ and $n_0^{(i)} = 1$.

Quantumness of an arbitrary state ρ can be defined [9] as the (Hilbert-Schmidt) distance to the convex set \mathcal{C} . Namely, the quantumness $Q(\rho)$ is given by

$$Q(\rho) = \min_{\rho_c \in \mathcal{C}} \|\rho - \rho_c\|, \quad (7)$$

where $\|A\| = \sqrt{\text{tr}(A^\dagger A)}$ is the Hilbert-Schmidt norm. In the following we will refer to $Q(\rho)$ simply as ‘‘the quantumness,’’ keeping in mind that other measures of quantumness can be defined; see, e.g., [14]. It has the natural properties that $Q(\rho) \geq 0$ for all ρ with equality for classical states ρ , and $Q(\rho)$ is a convex function of ρ . Using Eq. (3), one can show that the quantumness can be re-expressed in terms of Bloch matrices as

$$Q(\rho) = \frac{1}{2} \min_{W \text{ classical}} \|X - W\|, \quad (8)$$

where X is the Bloch matrix of ρ and W is given by (6).

In [6], a necessary and sufficient criterion for classicality in the spin-1 case was obtained. A spin-1 state is classical if and only if the 3×3 matrix Z defined (using the present notation) by $Z_{ab} = X_{ab} - X_{a0} X_{b0}$, with $1 \leq a, b \leq 3$, is positive semidefinite. Remarkably, the matrix Z is nothing but the Schur complement of the 1×1 upper left block of matrix X (note that $X_{00} = 1$). Therefore positive semidefiniteness of Z is equivalent to positive semidefiniteness of X . In other words, a spin-1 state is classical if and only if its matrix X is positive semidefinite. Equivalently, a spin-1 state is quantum if and only if the smallest eigenvalue of its matrix X is negative.

The Bloch matrix thus provides a simple classicality criterion. In the case of pure states, it also allows one to obtain an exact expression for the quantumness measure defined in Eq. (7). This is the goal of the next section.

III. PURE STATES

Starting from a one-dimensional parametrization of pure states, we now prove a lower bound to the minimization problem (7) and then show that this lower bound can be reached

by a classical state. This gives an analytic expression for Q for all pure states.

A. Parametrization

The Majorana representation [27,28] allows one to uniquely map any pure spin- j state to $2j$ points on the Bloch sphere. If the pure state undergoes a unitary transformation $e^{i\varphi\mathbf{J}\cdot\mathbf{n}}$ that represents a rotation of angle φ about vector \mathbf{n} then the Majorana points are rotated rigidly by that rotation. Under such a transformation, coherent states are rotated into coherent states, so that from its definition it is clear that quantumness is invariant under rotation of the coordinate system. Moreover, since X transforms under rotations as explained in Sec. II A, its eigenvalues are unchanged under such rotations.

The Majorana representation of a spin-1 pure state $|\psi\rangle$ just consists of two points on the unit sphere. These points correspond, via the stereographic projection $z = \cot \frac{\theta}{2} e^{i\phi}$, to the roots of the Majorana polynomial $P(z) = d_1 - \sqrt{2}d_0z + d_{-1}z^2$, with d_m , $-1 \leq m \leq 1$, the coefficients of the state $|\psi\rangle$ in the $|j,m\rangle$ basis. The sphere (or the spin-1 state) can always be rotated in such a way that these two Majorana points are brought to a canonical position where they have spherical coordinates $(\theta, \phi) = (\gamma, 0)$ and $(\pi - \gamma, 0)$ without changing the quantumness. States with Majorana points at positions $(\gamma, 0)$ and $(\pi - \gamma, 0)$ are given (up to normalization \mathcal{N}) by

$$|\psi_\gamma\rangle = \mathcal{N} \left(|1, -1\rangle + \frac{\sqrt{2}}{\sin \gamma} |1, 0\rangle + |1, 1\rangle \right), \quad (9)$$

with $\gamma \in [0, \pi/2]$ (see Fig. 1). We will use this expression as a canonical form for spin-1 pure states. The corresponding Bloch matrix X is given by

$$X = \begin{pmatrix} 1 & \sqrt{1-\lambda^2} & 0 & 0 \\ \sqrt{1-\lambda^2} & 1 & 0 & 0 \\ 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & \lambda \end{pmatrix}, \quad (10)$$

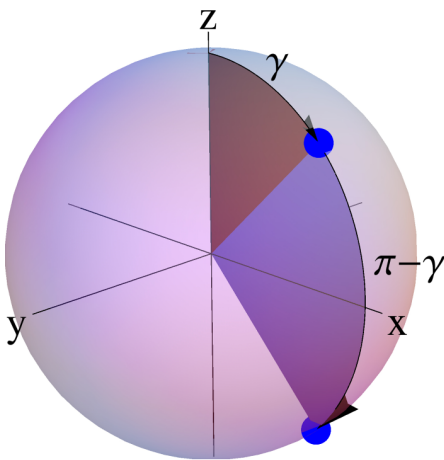


FIG. 1. The Majorana representation of the pure state $|\psi_\gamma\rangle$ given through Eq. (9), shown for $\gamma = \frac{\pi}{4}$, which corresponds to $\lambda = -\frac{1}{3}$.

with

$$\lambda = \frac{\sin^2 \gamma - 1}{\sin^2 \gamma + 1}. \quad (11)$$

The eigenvalues of X are $\pm\lambda$ and $1 \pm \sqrt{1 - \lambda^2}$. When γ varies in $[0, \pi/2]$, λ varies in $[-1, 0]$, so that the smallest eigenvalue (and the only negative one) is λ . We will use λ as the parameter for spin-1 pure states.

According to the criterion of Sec. II B, a state ρ is classical if and only if X is positive semidefinite, that is, if and only if $\lambda \geq 0$. For pure states, since $\lambda \in [-1, 0]$ this implies that $\lambda = 0$. The Bloch matrix (10) then corresponds to the Bloch matrix of a coherent state with vector $\mathbf{n} = (1, 0, 0)$. Another way of seeing this is to note that $\lambda = 0$ is equivalent to $\gamma = \pi/2$, which corresponds to both Majorana points coinciding, i.e., a coherent state. We recover the known fact that the only classical pure states are coherent states.

B. Lower bound for the full range

We now show that for an arbitrary pure state $|\psi\rangle$ whose Bloch matrix X has smallest eigenvalue λ , quantumness is such that

$$Q(|\psi\rangle) \geq -\sqrt{\frac{3}{8}}\lambda. \quad (12)$$

Without loss of generality, the quantumness of $|\psi\rangle$ can be calculated by first transforming it to the canonical form (9). Then we write the quantumness (8) as

$$Q(|\psi\rangle) = \frac{1}{2} \min_{W \text{ classical}} \sqrt{\sum_{\mu\nu=0}^3 (X_{\mu\nu} - W_{\mu\nu})^2}, \quad (13)$$

with W of the form (6) and X given by (10). In order to obtain (12) it is sufficient to show that $\sum_{\mu\nu} (X_{\mu\nu} - W_{\mu\nu})^2 \geq \frac{3}{2}\lambda^2$ for all classical states W . This is possible by proving

$$(X_{\mu\nu} - W_{\mu\nu})^2 \geq 0, \quad (14)$$

$$(X_{33} - W_{33})^2 - \lambda^2 \geq 0, \quad (15)$$

$$(X_{11} - W_{11})^2 + (X_{22} - W_{22})^2 - \frac{\lambda^2}{2} \geq 0. \quad (16)$$

The first claim is true for all μ, ν , since the entries of X and W are real numbers. Using (10), condition (15) can be rewritten as

$$(|\lambda| + W_{33})^2 - \lambda^2 \geq 0, \quad (17)$$

which obviously holds since $W_{33} = \sum_i w_i \cos^2 \theta_i \geq 0$. In order to prove (16), we define $a = (W_{11} + W_{22})$ and $b = (W_{11} - W_{22})$. Then one can show the identity,

$$\begin{aligned} & (X_{11} - W_{11})^2 + (X_{22} - W_{22})^2 - \frac{\lambda^2}{2} \\ &= \frac{1}{2} [(1-a)^2 - 2\lambda(1-a) + (\lambda+1-b)^2]. \end{aligned} \quad (18)$$

Noting that $a = \sum_i w_i \sin^2 \theta_i \in [0, 1]$ and $\lambda \leq 0$, it immediately follows that this quantity is non-negative, which completes the proof of (12).

C. Exact value of $Q(|\psi\rangle)$ for $\lambda \in [-1, -\frac{1}{2}]$

It turns out that in the parameter range $\lambda \in [-1, -\frac{1}{2}]$ there is a classical state at precisely the distance given by the lower bound (12). We consider the family of states of the form,

$$\rho_c(w, \beta) = (1 - 2w) \left| \frac{\pi}{2}, 0 \right\rangle \left\langle \frac{\pi}{2}, 0 \right| + w \left| \frac{\pi}{2}, \beta \right\rangle \left\langle \frac{\pi}{2}, \beta \right| + w \left| \frac{\pi}{2}, -\beta \right\rangle \left\langle \frac{\pi}{2}, -\beta \right|, \quad (19)$$

which are classical by construction for $w \in [0, 1/2]$, since they are a mixture of coherent states $|\theta, \phi\rangle$. By calculating the unconstrained minimum,

$$\min_{w, \beta} |||\psi\rangle\langle\psi| - \rho_c(w, \beta)||, \quad (20)$$

the optimal choices for the parameters w and β are found to be

$$w = \frac{(4\lambda + 2)(1 - \sqrt{1 - \lambda^2}) - \lambda^2}{17\lambda + 8}, \quad (21)$$

and

$$\beta = \arccos\left(\frac{-\sqrt{1 - \lambda^2} - 2\lambda - 1}{2\lambda}\right). \quad (22)$$

The condition $w \in [0, 1/2]$ translates to $\lambda \leq -1/2$. For these values the Bloch matrix of the state (19) reduces to

$$W = \begin{pmatrix} 1 & \sqrt{1 - \lambda^2} & 0 & 0 \\ \sqrt{1 - \lambda^2} & 1 + \frac{\lambda}{2} & 0 & 0 \\ 0 & 0 & -\frac{\lambda}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (23)$$

Note that since the set of classical states is closed and convex [6], there is a unique closest state to any given state for the (Euclidean) Hilbert-Schmidt distance. Since the distance from the state W to the state X (10) is exactly the value of the lower bound, it shows that W represents the closest classical state (ccs) for $|\psi\rangle$ in the range of $\lambda \in [-1, -\frac{1}{2}]$.

If $\lambda > -\frac{1}{2}$ the state corresponding to (23) does not represent a quantum state any more, since the corresponding density matrix is no longer positive. Actually, in the next section we find a tighter lower bound for $\lambda \in]-\frac{1}{2}, 0]$, which in particular implies that the distance between a quantum state and the set \mathcal{C} is larger than $\sqrt{3/8}|\lambda|$ for $\lambda \in]-\frac{1}{2}, 0]$. This proves that no classical state exists in this range $\lambda \in]-\frac{1}{2}, 0]$ that saturates the bound (12).

D. Tighter bound in the range $\lambda \in]-\frac{1}{2}, 0]$

In this section we show that for $\lambda \in]-\frac{1}{2}, 0]$ one has

$$Q(|\psi\rangle) \geq \frac{1}{2}\sqrt{\lambda^2 + \ell(\lambda)}, \quad (24)$$

where $\ell(\lambda)$ is given by

$$\ell(\lambda) = \frac{1}{216} \left[3h^5 \sqrt{\frac{1 - \lambda}{(\lambda + 1)^3}} - \frac{6h^2(\lambda^2 - 52\lambda + 55)}{\lambda + 1} + h^4 - 216h\sqrt{1 - \lambda^2} + 72(11 - 4\lambda^2 + 4\lambda) \right], \quad (25)$$

with

$$h = 6^{1/3} [9\sqrt{1 - \lambda^2} + \sqrt{3(\lambda + 1)(25 - 31\lambda - 2\lambda^2)}]^{1/3}. \quad (26)$$

The bound (24) is tighter than the one obtained in Sec. III B, as can be shown by proving that over the range $\lambda \in]-\frac{1}{2}, 0]$ one has

$$\frac{\sqrt{\lambda^2 + \ell(\lambda)}}{2} > -\sqrt{\frac{3}{8}}\lambda \quad (27)$$

(see end of the Appendix).

In order to prove the lower bound (24) it is sufficient to show that $\sum_{\mu\nu} (X_{\mu\nu} - W_{\mu\nu})^2 \geq \lambda^2 + \ell(\lambda)$ for all classical states. This is possible by proving

$$(X_{\mu\nu} - W_{\mu\nu})^2 \geq 0, \quad (28)$$

$$(X_{33} - W_{33})^2 - \lambda^2 \geq 0, \quad (29)$$

$$(X_{11} - W_{11})^2 + (X_{22} - W_{22})^2 + 2(X_{01} - W_{01})^2 \geq \ell(\lambda). \quad (30)$$

Conditions (28) and (29) were already proven in the previous section, so we only have to show (30). This can be done by analytically calculating the minimal value of the left-hand side of (30) under the restrictions on the values of $W_{\mu\nu}$ implied by Eq. (6). For readability, we rewrite the left-hand side of (30), using the form (10) for a general pure state Bloch matrix X and Eq. (6) for a general classical state W as

$$F(u, v, g) := (1 - u)^2 + (\lambda + v)^2 + 2(\sqrt{1 - \lambda^2} - g)^2, \quad (31)$$

with $u = \sum_i w_i \sin^2 \theta_i \cos^2 \phi_i$, $v = \sum_i w_i \sin^2 \theta_i \sin^2 \phi_i$, and $g = \sum_i w_i \sin \theta_i \cos \phi_i$. These new variables are such that

$$u + v \leq 1, \quad u, v \geq 0 \\ -\sqrt{u} \leq g \leq \sqrt{u}. \quad (32)$$

The last condition is derived from Jensen's inequality $(\sum_i w_i a_i)^2 \leq \sum_i w_i a_i^2$ with $a_i = \sin \theta_i \cos \phi_i$. The minimum of $F(u, v, g)$ under the constraints (32) can be calculated analytically, and, as shown in the Appendix, it is equal to $\ell(\lambda)$ given in (25). This proves Eq. (30), and thereby the tighter lower bound (24) for the range $\lambda \in]-\frac{1}{2}, 0]$.

E. Exact value of $Q(|\psi\rangle)$ for $\lambda \in]-\frac{1}{2}, 0]$

The tighter lower bound (24) can be reached in the range of $\lambda \in]-\frac{1}{2}, 0]$, since there are classical states at this distance. Using a similar approach as in Sec. III C, we consider a family of classical states of the form,

$$\rho_c(\beta) = \frac{1}{2} \left(\left| \frac{\pi}{2}, \beta \right\rangle \left\langle \frac{\pi}{2}, \beta \right| + \left| \frac{\pi}{2}, -\beta \right\rangle \left\langle \frac{\pi}{2}, -\beta \right| \right), \quad (33)$$

which are a mixture of just two coherent states $|\theta, \phi\rangle$ with equal weights $\frac{1}{2}$. Let a pure state $|\psi\rangle$ have a Bloch matrix with smallest eigenvalue λ . The state $\rho_c(\beta)$ closest to the canonical form (9) of $|\psi\rangle$ is determined by the condition,

$$\frac{\partial}{\partial \beta} |||\psi\rangle\langle\psi| - \rho_c(\beta)|| = 0, \quad (34)$$

which has the solution $\beta = \arccos d$, with d defined as the real root of the polynomial,

$$P(y) = \sqrt{1 - \lambda^2} + y(1 + \lambda) - 2y^3, \quad (35)$$

where $\lambda \in] -\frac{1}{2}, 0]$, corresponding to $d \in] \frac{\sqrt{3}}{2}, 1]$. Using this value of β gives the Bloch matrix of ρ_c as

$$W = \begin{pmatrix} 1 & d & 0 & 0 \\ d & d^2 & 0 & 0 \\ 0 & 0 & 1 - d^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (36)$$

The state represented by (36) is then exactly at the distance to the pure state (10) given by the tighter lower bound (24). Therefore we have proven that the classical state closest to (10) is (36) for the parameter range $\lambda \in] -\frac{1}{2}, 0]$.

F. Summary of results for pure states

To conclude, let an arbitrary pure spin-1 state $|\psi\rangle$ be given by its Bloch matrix (2). If the smallest eigenvalue of X is denoted by λ , then the quantumness of $|\psi\rangle$ is equal to the quantumness of a state with Bloch matrix (10), and takes the form,

$$Q(|\psi\rangle) = f(\lambda), \quad (37)$$

with

$$f(\lambda) := \begin{cases} -\sqrt{\frac{3}{8}}\lambda & \text{for } \lambda \leq -\frac{1}{2}, \\ \frac{1}{2}\sqrt{\lambda^2 + \ell(\lambda)} & \text{for } \lambda > -\frac{1}{2}, \end{cases} \quad (38)$$

and $\ell(\lambda)$ given by Eq. (25). The function $f(\lambda)$ is shown in Fig. 2. It is continuous at $\lambda = -\frac{1}{2}$. At this plot scale, $f(\lambda)$ is almost indistinguishable from a linear function. The maximal difference between $f(\lambda)$ and $-\sqrt{\frac{3}{8}}\lambda$ is less than 0.0016 over the interval $[-1, 0]$.

The classical states closest to a pure state $|\psi\rangle$ take a different expression in the two regions $\lambda < -\frac{1}{2}$ and $\lambda > -\frac{1}{2}$, respectively, given by (23) and (36). A video showing how the closest classical states vary as a function of the pure states is given in the Supplemental Material [29]. In contrast to the

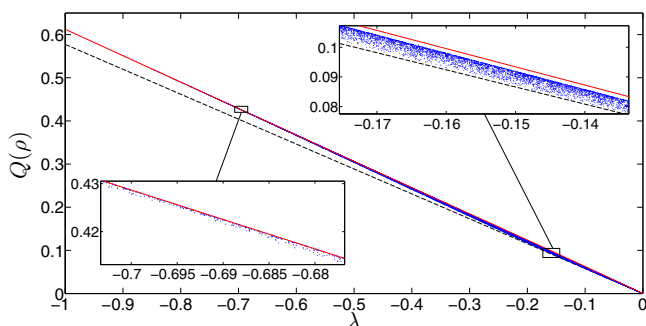


FIG. 2. Quantumness of randomly generated mixed states, as a function of the smallest eigenvalue of their Bloch matrix. There are 50 000 points, each one corresponding to a random state. Red line corresponds to the pure state analytic result $f(\lambda)$ given by Eq. (38). Dashed line indicates the lower bound (45). Function $f(\lambda)$ appears to be an upper bound on the quantumness of mixed states (see inset).

case of the queen of quantum for $j = 1$, corresponding to $\lambda = -1$ [9], these closest classical states (ccs) are not simply a mixture of the pure state $|\psi\rangle$ itself and the maximally mixed state, i.e., for $\lambda \neq -1$,

$$\text{ccs} \neq a|\psi\rangle\langle\psi| + (1-a)\frac{\mathbb{1}}{3}, \quad 0 \leq a \leq 1. \quad (39)$$

IV. MIXED STATES

A. Mixed state quantumness

For pure states we obtained the analytical expression (37) for quantumness as a function of a single parameter, namely the smallest eigenvalue λ of the Bloch matrix of the state. In this section we investigate the dependence of $Q(\rho)$ as a function of λ for mixed states. For a given state ρ the quantumness can be obtained numerically by determining the closest classical state of ρ . To find this state we randomly generate a large sample of coherent states $\{|\theta_i, \phi_i\rangle\}$ defined through Eq. (5), and then optimize the weights w_i of this decomposition,

$$\rho_c = \sum_i w_i |\theta_i, \phi_i\rangle\langle\theta_i, \phi_i|, \quad (40)$$

so that the distance from ρ to ρ_c is minimal. As the function Q^2 defined in (7) corresponds to the minimization of a function which is quadratic in the w_i , this optimization can be done by quadratic programming. The result of the optimization yields an approximation of the quantumness: In general it is overestimated by this approach, as coherent states appearing in the decompositions of the closest classical state may not be included in our random sample. The overestimation incurred by the numerical approach can be estimated by considering pure states, for which the analytical expression (37) is available. For these states the overestimation is typically of the order of $\sim 10^{-6}$ for the numerical parameters used in the paper. For mixed states, the overestimation can be probed, for instance, by increasing the number of coherent states involved in the sum (40), or by changing the choice of coherent states in the random list. The results obtained are quite independent on increasing the number of coherent states over which we optimize.

In Fig. 2 we plot the quantumness of mixed states as a function of the smallest eigenvalue of their Bloch matrix. Since, from the classicality criterion $X \geq 0$, nonclassical states are such that $\lambda \in [-1, 0]$, we restrict our plot to this interval (note that for classical states λ takes positive values, while the quantumness is zero by definition). The mixed states were randomly generated from the Hilbert-Schmidt ensemble of matrices $\rho = AA^\dagger / \text{tr}(AA^\dagger)$, with A a complex matrix with independent Gaussian entries (see [30] for detail). All points lie very close to the pure state result. This signifies that quantumness of a mixed state appears to largely depend on a single parameter, which is the smallest eigenvalue of its Bloch matrix, although mixed states cannot be reduced to a one-parameter family (as is the case for pure states, up to rotations).

B. Upper bound for quantumness of mixed states

We conjecture that the function f provides an upper bound for the quantumness of mixed states, namely,

$$Q(\rho) \leq f(\lambda), \quad (41)$$

with λ the smallest eigenvalue of the Bloch matrix of ρ . This conjecture is supported by strong numerical evidence as shown in the inset of Fig. 2. More precisely, Fig. 3 displays the difference between the quantumness and $f(\lambda)$ as a function of the smallest eigenvalue of the Bloch matrix. In fact, we were not able to find a single state which violates the bound. It may happen that, for states very close to pure states, the numerical overestimation of quantumness due to our optimization procedure leads to a result larger than $f(\lambda)$; however, by increasing the accuracy of our estimation [that is, taking more coherent states in the sum (40)], we were always able to get this estimate back below the threshold $f(\lambda)$. Numerical evidence thus suggests that this upper bound is valid for all mixed states. Note that the true value of the quantumness can only be smaller than the numerical estimate, as there is at least one classical state at the corresponding distance.

The almost empty region in the upper right corner of Fig. 3 (visible also just below the upper bound in the upper inset of Fig. 2) corresponds to the region between $f(\lambda)$ and the straight line $-\sqrt{3/8}\lambda$ in the interval $[-\frac{1}{2}, 0]$. This apparent emptiness just comes from our numerical sampling: Indeed, this region can be filled, e.g., by points corresponding to mixed states of the form,

$$\rho = a|\psi\rangle\langle\psi| + (1-a)\text{ccs}(|\psi\rangle), \quad (42)$$

with $0 \leq a \leq 1$ and $|\psi\rangle$ a pure state with closest classical state $\text{ccs}(|\psi\rangle)$ and $\lambda \in [-\frac{1}{2}, 0]$.

In the special case where a mixed state ρ can be written as a convex combination of a pure state and its closest classical state ccs , as in (42), Eq. (41) can be proven. This can be shown by the fact that $\|\rho - \text{ccs}(|\psi\rangle)\| = aQ(|\psi\rangle)$, so that $Q(\rho) \leq af(\lambda_\psi)$, with λ_ψ the smallest eigenvalue of the Bloch matrix of $|\psi\rangle$. By using the explicit form of f given by (38), one can show that $af(\lambda_\psi) \leq f(a\lambda_\psi)$, for $0 \leq a \leq 1$ (this is true for $-1 \leq \lambda \leq -1/2$ because of the inequality (27), and for $-1/2 \leq \lambda \leq 0$ by concavity of f over this interval). From the forms (10) and (23),(36) of the Bloch matrices, one can show that for states (42) the smallest eigenvalue of the Bloch

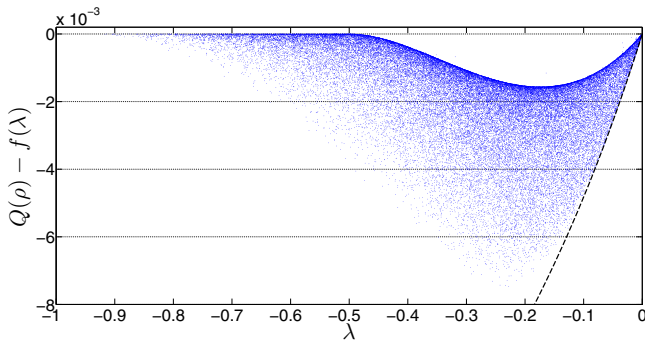


FIG. 3. Difference between the quantumness and the hypothetical upper bound $f(\lambda)$ as a function of the smallest eigenvalue of the Bloch matrix (same data as in Fig. 2). The difference between the upper bound and the quantumness is of the order of 10^{-3} . The numerical error is of order 10^{-6} , and our numerical procedure can only overestimate quantumness so that the points could only be lower than they appear here by that amount. The dashed line corresponds to the lower bound (45).

matrix of ρ is given by $\lambda = a\lambda_\psi$, hence (41). This proves the upper bound for the family of states (42). However, a proof for arbitrary mixed states is still missing.

C. Lower bound for quantumness of mixed states

The quantumness of mixed states can be bound from below by minimizing over a larger set than in Eq. (8) (see [25] for a similar approach). Let X be the Bloch matrix of some state ρ and λ be the smallest eigenvalue of X . A lower bound can be obtained as

$$\frac{1}{2} \min_{W \text{ classical}} \|X - W\| \geq \frac{1}{2} \min_{\tilde{W}, \tilde{X}} \|\tilde{X} - \tilde{W}\|, \quad (43)$$

where \tilde{W} runs over all positive semidefinite matrices with $\text{tr}\tilde{W} = 2$, and \tilde{X} runs over all real symmetric matrices with one eigenvalue equal to λ and $\text{tr}\tilde{X} = 2$. Furthermore, we can write \tilde{X} in its diagonal form $\tilde{X} = \text{diag}(x_1, x_2, x_3, \lambda)$ with x_i arbitrary real numbers since the norm and the set over which \tilde{W} runs in the right-hand side of Eq. (43) are invariant under orthogonal transformations.

Because \tilde{X} is diagonal the optimal \tilde{W} will also be in diagonal form. Since \tilde{W} is positive, let $\tilde{W} = \text{diag}(w_1^2, w_2^2, w_3^2, w_4^2)$, with real w_i such that $\sum_{i=1}^4 w_i^2 = 2$. The right-hand side of (43) can then be rewritten as

$$\frac{1}{2} \min_{\substack{x_i, w_i \in \mathbb{R} \\ \sum_{i=1}^3 x_i = 2 - \lambda \\ \sum_{i=1}^4 w_i^2 = 2}} \left[(\lambda - w_4^2)^2 + \sum_{i=1}^3 (x_i - w_i^2)^2 \right]^{1/2}. \quad (44)$$

This is a simple problem of minimization under constraints, which can be solved by introducing appropriate Lagrange multipliers. When λ is negative (nonclassical states), the critical points of the Lagrange function are found to be such that either $w_i = 0$ for $1 \leq i \leq 3$, or $w_4 = 0$. The latter case yields the smallest value for the quantumness, which is equal to $-\frac{\lambda}{\sqrt{3}}$. So the quantumness of any mixed state ρ with smallest eigenvalue λ of its Bloch matrix is bound by

$$Q(\rho) \geq -\frac{\lambda}{\sqrt{3}}. \quad (45)$$

This lower bound corresponds to the dashed line in Figs. 2 and 3. For small enough quantumness, the two bounds provided in this section are close to tight in the sense that the quantumness of random mixed states extends almost over the whole range between them.

V. CONNECTION WITH ENTANGLEMENT

We now establish a connection between quantumness and entanglement, and relate the smallest eigenvalue of the Bloch matrix to known entanglement measures such as the negativity and the concurrence.

A. Entanglement

A bipartite pure state $|\psi\rangle$ is called separable if it can be written as a direct product of pure states of its subsystems,

$$|\psi\rangle = |\psi^{(1)}\rangle \otimes |\psi^{(2)}\rangle. \quad (46)$$

This definition can be extended to mixed states: A bipartite mixed state is called separable if it can be written as a convex sum of tensor products of quantum states of the subsystems,

$$\rho = \sum_i w_i \rho_i^{(1)} \otimes \rho_i^{(2)}, \quad (47)$$

where the w_i are classical probabilities with $w_i \geq 0$ and $\sum_i w_i = 1$. If a state cannot be written in this form then it is called entangled [31].

For two spin- $\frac{1}{2}$ states, entanglement can be detected by use of the partial transpose [32]. The necessary and sufficient ‘‘positive partial transpose’’ (PPT) criterion [33] states that a state of two spins- $\frac{1}{2}$ (or a spin- $\frac{1}{2}$ and a spin-1) is separable if and only if ρ^{PT} is positive semidefinite, where PT denotes the partial transpose operation. For higher spins there exist PPT entangled states [17,34].

In order to quantify entanglement, commonly used measures are the negativity and the concurrence. The negativity is given as

$$\mathcal{N}(\rho) = \sum_i \frac{|\mu_i| - \mu_i}{2}, \quad (48)$$

where μ_i are the eigenvalues of ρ^{PT} . The concept of negativity is also connected to the concept of robustness of entanglement [35].

The concurrence C was developed as an analytic solution of the entanglement of formation for two spins- $\frac{1}{2}$ [36]. For a two spin- $\frac{1}{2}$ state ρ it is given as

$$C(\rho) = \max\{0, \tau_1 - \tau_2 - \tau_3 - \tau_4\}, \quad (49)$$

where τ_i are the square roots of the eigenvalues of the matrix,

$$\rho(\sigma_y \otimes \sigma_y) \rho^*(\sigma_y \otimes \sigma_y), \quad (50)$$

in decreasing order, and $*$ denotes the complex conjugation. In Sec. VC we will relate these entanglement measures with quantumness. We first discuss the analogy between classicality and separability.

B. Classicality and separability

Classicality is a property defined for a spin- j state. It is interesting to look at a spin- j state as the projection of a tensor product of $2j$ spin- $\frac{1}{2}$ states onto the subspace symmetric under permutation of the particles. Any basis vector $|j, m\rangle$ then appears as a symmetrized $2j$ -fold tensor product.

The subspace of pure symmetric states of two spins- $\frac{1}{2}$ is spanned by the Dicke states,

$$|D_0\rangle = |\uparrow\uparrow\rangle, \quad |D_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad |D_2\rangle = |\downarrow\downarrow\rangle. \quad (51)$$

The basis vector $|1, m\rangle$ corresponds to $|D_{1-m}\rangle$ for $-1 \leq m \leq 1$. There is a difference between mixed symmetric states and symmetric mixtures of states. The former are defined as mixtures of pure symmetric states and arise from the physics of indistinguishable particles; the latter correspond to symmetrically mixing arbitrary states, i.e., a purely classical

symmetrization procedure. For example, consider the state,

$$\rho = \frac{1}{2} |\alpha\rangle\langle\alpha|^{j=1/2} \otimes |\alpha'\rangle\langle\alpha'|^{j=1/2} + \frac{1}{2} |\alpha'\rangle\langle\alpha'|^{j=1/2} \otimes |\alpha\rangle\langle\alpha|^{j=1/2}, \quad (52)$$

which is mixture of two distinct spin- $\frac{1}{2}$ coherent states $|\alpha\rangle^{j=1/2}$ and $|\alpha'\rangle^{j=1/2}$. Such a state is a symmetric mixture, but not a mixed symmetric state.

We now show that the set of two-qubit symmetric separable states is identical to the set of classical spin-1 states. First, spin-coherent states are separable: Identifying (in $|j, m\rangle$ notation) $|\frac{1}{2}, \frac{1}{2}\rangle = |\uparrow\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle = |\downarrow\rangle$, the tensor product of two identical spin- $\frac{1}{2}$ coherent states (5) is

$$\begin{aligned} & \left(\cos \frac{\theta}{2} |\uparrow\rangle + \sin \frac{\theta}{2} e^{-i\phi} |\downarrow\rangle \right)^{\otimes 2} \\ &= \cos^2 \frac{\theta}{2} |D_0\rangle + \sqrt{2} \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{-i\phi} |D_1\rangle \\ &+ \sin^2 \frac{\theta}{2} e^{-2i\phi} |D_2\rangle, \end{aligned} \quad (53)$$

which, from the correspondence $|1, m\rangle = |D_{1-m}\rangle$, is equivalent to

$$|\alpha\rangle^{j=\frac{1}{2}} \otimes |\alpha\rangle^{j=\frac{1}{2}} = |\alpha\rangle^{j=1}, \quad (54)$$

where $|\alpha\rangle^j$ is a spin- j coherent state given by (5). Thus the spin-1 coherent states are separable in the tensor product space. Therefore, all classical states of the form (4), as mixtures of coherent states, can be identified with separable states.

Conversely, a two qubit symmetric separable state $\rho_s = \sum_i w_i \rho_i^{(1)} \otimes \rho_i^{(2)}$ with $w_i > 0$ can be identified with a classical spin-1 state. Indeed, if ρ_s is symmetric then

$$\langle D^- | \rho_s | D^- \rangle = 0, \quad (55)$$

with $|D^- \rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. This is equivalent to

$$\sum_i w_i \langle D^- | \rho_i^{(1)} \otimes \rho_i^{(2)} | D^- \rangle = 0. \quad (56)$$

Since all summands are non-negative (by positivity of density matrices) it follows that

$$\langle D^- | \rho_i^{(1)} \otimes \rho_i^{(2)} | D^- \rangle = 0 \quad \forall i. \quad (57)$$

If the qubit states $\rho^{(1,2)}$ are written with the Bloch vectors $\mathbf{X}^{(1,2)}$ according to Eq. (1), direct calculations give

$$\langle D^- | \rho_i^{(1)} \otimes \rho_i^{(2)} | D^- \rangle = \frac{1}{4} (1 - \mathbf{X}^{(1)} \cdot \mathbf{X}^{(2)}). \quad (58)$$

Because the Bloch vectors are such that $\|\mathbf{X}^{(1,2)}\| \leq 1$, Eq. (58) implies that $\mathbf{X}^{(1)} = \mathbf{X}^{(2)}$ and $\|\mathbf{X}^{(1,2)}\| = 1$. Thus $\rho_i^{(1)} = \rho_i^{(2)}$, which corresponds to the same pure qubit state $|\alpha_i\rangle\langle\alpha_i|^{j=1/2}$. Therefore one can write

$$\rho_s = \sum_i w_i |\alpha_i\rangle\langle\alpha_i|^{j=1/2} \otimes |\alpha_i\rangle\langle\alpha_i|^{j=1/2}. \quad (59)$$

With (54) it follows that ρ_s can be identified with

$$\sum_i w_i |\alpha_i\rangle\langle\alpha_i|^{j=1}, \quad (60)$$

which represents a classical state (4). Thus, the set of classical spin-1 states can be identified with the set of separable symmetric states of two qubits. Note that in the context of quantum optics, there have been attempts to unify several notions of quantumness; see e.g., [37–39].

This equivalence can also be shown indirectly using the PPT criterion. Indeed, there is a remarkable connection between the partial transpose of a state ρ and the Bloch matrix X of ρ . Namely, one can easily check that

$$\rho^{\text{PT}} = \frac{1}{2} R X R^\dagger, \quad (61)$$

with the unitary matrix,

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -i & 0 \\ 0 & 1 & i & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix}. \quad (62)$$

Therefore, the Bloch matrix is nothing but the partial transpose of ρ expressed in a different basis. As shown in Sec. II B, a necessary and sufficient condition for classicality is that X be positive semidefinite. As the eigenvalues are unchanged by the change of basis (61) (but for a factor $\frac{1}{2}$), this condition is equivalent to the positive semidefiniteness of ρ^{PT} , which in turn is equivalent to separability. In other words, this proves that a spin-1 state is entangled (when seen as a bipartite system) if and only if its quantumness is nonzero.

Any separable state can be written in the form (47), with possibly $\rho_i^{(1)} \neq \rho_i^{(2)}$. If that state lies in the subspace spanned by (51), then necessarily, from the considerations above, $\rho_i^{(1)} = \rho_i^{(2)}$, so that ρ can be cast in the form,

$$\rho = \sum_i w_i \rho_i \otimes \rho_i, \quad (63)$$

with ρ_i spin- $\frac{1}{2}$ coherent states. This shows that spin-1 classical states are at the same time mixtures of symmetric bipartite spin-1/2 states and symmetric mixtures of the form (63).

C. Quantumness and entanglement

In Secs. III and IV we related quantumness of a state ρ to the smallest eigenvalue of its Bloch matrix (2). If this smallest eigenvalue is denoted by λ , then from the correspondence (61), the smallest eigenvalue of ρ^{PT} is equal to $\lambda/2$. In the case of a bipartition of two spin- $\frac{1}{2}$ states, ρ^{PT} has at most one negative eigenvalue [40], so that negativity (48) reduces to $\mathcal{N}(\rho) = -\lambda/2$. In the case of pure states, the concurrence defined in (49) reduces to

$$C(|\psi\rangle\langle\psi|) = -\lambda. \quad (64)$$

Of course, as is expected for pure states, the negativity and the concurrence are simply related by $C(|\psi\rangle\langle\psi|) = 2\mathcal{N}(|\psi\rangle\langle\psi|)$ [40].

The function $f(\lambda)$ defined in (38) thus allows us to express quantumness as a function of negativity for pure spin-1 states. For mixed spin-1 states Eq. (41) becomes

$$d_{\text{HS}}(\rho, \mathcal{C}) \leq f(-2\mathcal{N}(\rho)), \quad (65)$$

and as we showed equality holds for pure states. Furthermore, it gives an insight into the geometry of entangled states as

it allows one to connect negativity to a geometric property, namely the Hilbert-Schmidt distance d_{HS} from an entangled state to the set \mathcal{C} of symmetric separable states. In general, since the closest separable state found in [25] is nonsymmetric, the corresponding minimal Hilbert-Schmidt distance obtained in [25] is smaller than the one we get as we consider the distance to symmetric separable states only.

VI. CONCLUSION

In this paper we investigated the quantumness of spin-1 states, defined as Hilbert-Schmidt distance to the convex set of classical spin-1 states. We found the analytical solution for the quantumness $Q(|\psi\rangle)$ of arbitrary pure states. It can be expressed as a function of the smallest eigenvalue of the Bloch matrix associated with $|\psi\rangle$. For mixed states, the same function appears to give an upper bound for $Q(\rho)$ according to extensive numerical investigations. We established the connection of $Q(\rho)$ with entanglement measures.

The closest classical state also provides a classicality witness, in the spirit of [41]. Our derivations provide another example of the usefulness of the tensor representation of spin states [26].

Spin-1 states have important physical applications. For instance, there is a connection between spin-1 states and two-photon states. De la Hoz *et al.* showed that unpolarized two-photon states correspond to the states of maximal quantumness, i.e., the states given by Eq. (10) with $\lambda = -1$ [42–44]. Our findings might therefore become important for improving the understanding of the quantum properties of the polarization of light.

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APPENDIX: ANALYTIC CALCULATION OF THE MINIMA

Here we will calculate the minimal value of F defined in (31) under the constraints (32). If $\lambda = 0$, the minimum of F is zero. We exclude this case in the following for convenience and restrict ourselves to the interval $\lambda \in]-1/2, 0[$. We will use the fact that the minimal value of a function, restricted to a certain parameter range, has its minimal value either on a critical point or at the border of the parameter range. This will give a list of candidates for the global minimum. The smallest value in this list is then the global minimum.

To calculate the minimal value, we distinguish two cases, $u \geq 1 - \lambda^2$ and $u < 1 - \lambda^2$. In each case we can simplify the problem by setting the variable g to its optimal value. In the first case $D := F(g = \sqrt{1 - \lambda^2})$ so that the third term vanishes, and in the second case $E := F(g = \sqrt{u})$, which makes the last term as small as possible.

In both cases the new functions,

$$D = (1 - u)^2 + (\lambda + v)^2, \quad (A1)$$

$$E = (1 - u)^2 + (\lambda + v)^2 + 2(\sqrt{1 - \lambda^2} - \sqrt{u})^2, \quad (A2)$$

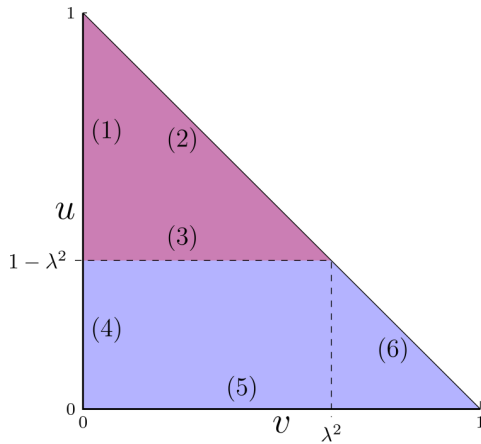


FIG. 4. Visualization of the allowed parameter range of the variables u and v . The upper area corresponds to $u \geq 1 - \lambda^2$, while the lower corresponds to $u \leq 1 - \lambda^2$. We call the function $F(u, v, g)$ restricted to the upper (lower) area D (E).

do not have critical points in the allowed parameter range of u and v (32), since $\nabla_{u,v} D = 0$ is only solved by $(u, v) = (1, -\lambda)$, which is outside the parameter range for $\lambda < 0$, and $\nabla_{u,v} E = 0$ is only solved by $(u, v) = (\sqrt[3]{1 - \lambda^2}, -\lambda)$, which is also outside the parameter range for $\lambda < 0$, since it contradicts the condition $u + v \leq 1$. Therefore both functions have to have their minimal value on the borders of the parameter range depicted in Fig. 4. The function D restricted to the line (1) in Fig. 4 will be referred to as D^1 , analogs D^2, D^3 . These three functions do not have a critical point on the interior of their respective parameter ranges, so the minimal value must be in all three cases on one of the two vertices. Consider the candidates for the minimal value for the function D , as

$$\left. \begin{array}{l} D^1(u = 1) \\ D^2(v = 0) \end{array} \right\} = \lambda^2, \quad (\text{A3})$$

$$\left. \begin{array}{l} D^1(u = 1 - \lambda^2) \\ D^3(v = 0) \end{array} \right\} = \lambda^4 + \lambda^2, \quad (\text{A4})$$

$$\left. \begin{array}{l} D^2(v = \lambda^2) \\ D^3(v = \lambda^2) \end{array} \right\} = \lambda^2(2\lambda^2 + 2\lambda + 1). \quad (\text{A5})$$

Comparing these values the minimal value of D is found to be $\lambda^2(2\lambda^2 + 2\lambda + 1)$.

The minimum of the function E will be calculated analogously. The function on the line (3) in Fig. 4 will be referred to

as E^3 , similar E^4 on line (4), and so forth. The function E^3 is the same as D^3 so its minimal value is also $\lambda^2(2\lambda^2 + 2\lambda + 1)$.

The function $E^4(u) = (1 - u)^2 + \lambda^2 + 2(\sqrt{1 - \lambda^2} - \sqrt{u})^2$ has a critical value at $u = \sqrt[3]{1 - \lambda^2}$, which is larger than $1 - \lambda^2$, and therefore outside the allowed range of the lower area in Fig. 4. So the minimal value is reached at the second of the two edges,

$$E^4(u = 0) = 3 - \lambda^2, \quad (\text{A6})$$

$$E^4(u = 1 - \lambda^2) = \lambda^4 + \lambda^2. \quad (\text{A7})$$

The function $E^5(v) = 1 + (v + \lambda)^2 + 2(1 - \lambda^2)$ has a critical value in the allowed parameter range, at $v = -\lambda$, corresponding to a minimum,

$$E^5(v = -\lambda) = 3 - 2\lambda^2. \quad (\text{A8})$$

The function $E^6(u) = (1 - u)^2 + (\lambda + 1 - u)^2 + 2(\sqrt{1 - \lambda^2} - \sqrt{u})^2$ has a critical value in the allowed parameter range of $u \in [0, 1 - \lambda^2]$. The condition $\partial_u E^6 = 0$ gives

$$1 + \lambda + \frac{\sqrt{1 - \lambda^2}}{\sqrt{u}} - 2u = 0, \quad (\text{A9})$$

with the substitution $u = y^2$ the optimal value of u is given through the real root d of

$$\sqrt{1 - \lambda^2} + y(1 + \lambda) - 2y^3 = 0, \quad (\text{A10})$$

which is the same polynomial as in (35). The second derivative,

$$\frac{\partial^2 E^6}{\partial u^2} = \frac{\sqrt{1 - \lambda^2}}{u^{3/2}} + 4, \quad (\text{A11})$$

is positive over the whole parameter range, so the critical point is a minimum, with the value,

$$\ell(\lambda) = E^6(u = d^2). \quad (\text{A12})$$

With this list of local minima, for all possible cases, the global minimum of (31) is found to be (A12), which yields (25).

Proving Eq. (27) is equivalent to showing that $\ell(\lambda) \geq \frac{\lambda^2}{2}$. We have $E^6 \geq \frac{\lambda^2}{2}$, since

$$E^6 - \frac{\lambda^2}{2} = 2(\sqrt{u} - \sqrt{1 - \lambda^2})^2 + \frac{1}{2}[\lambda + 2(1 - u)]^2, \quad (\text{A13})$$

which, as the sum of squares, is always non-negative. Therefore, the minimum of E^6 is also larger or equal to $\frac{\lambda^2}{2}$. As an immediate consequence, inequality (27) holds.

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A.2. Partial transpose criterion for symmetric states

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Partial transpose criteria for symmetric states

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We express the positive-partial-transpose (PPT) separability criterion for symmetric states of multiqubit systems in terms of matrix inequalities based on the recently introduced tensor representation for spin states. We construct a matrix from the tensor representation of the state and show that it is similar to the partial transpose of the density matrix written in the computational basis. Furthermore, the positivity of this matrix is equivalent to the positivity of a correlation matrix constructed from tensor products of Pauli operators. This allows for a more transparent experimental interpretation of the PPT criteria for an arbitrary spin- j state. The unitary matrices connecting our matrix to the partial transpose of the state generalize the so-called magic basis that plays a central role in Wootters' explicit formula for the concurrence of a two-qubit system and the Bell bases used for the teleportation of a one- or two-qubit state.

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I. INTRODUCTION

Quantum information provides a window on various remarkable features of quantum mechanics, such as entanglement [1] or teleportation [2]. A central resource in quantum information processing is quantum entanglement. A quantum state is said to be separable if it can be written as a convex sum of product states, i.e., states that are tensor products of states of all the subsystems; otherwise it is said to be entangled [3]. The state of a bipartite quantum system is known to be separable if and only if it remains positive under all positive quantum maps. Looking at a subclass of positive quantum channels, one obtains necessary conditions for separability, which therefore signal bipartite entanglement if the condition is violated. In this respect, a central role is played by the “positive-partial-transposed criterion” (PPT), physically obtained by time reversal of one of the two subsystems [4,5]. For systems with Hilbert-space dimensions at most 2×2 or 2×3 , PPT is also sufficient for separability. For higher dimensional systems, entangled states exist that have positive partial transpose [6,7].

For multipartite systems, the situation is substantially more complicated due to the possibility that only certain bipartitions could be entangled [8]. For three qubits, six different stochastic local operations and classical communication (SLOCC) - equivalence classes exist (i.e., families of states that can be transformed into each other with nonzero probability using only stochastic local operations and classical communication), including two of genuine multipartite entanglement [9,10]. For four qubits, there are already uncountably many SLOCC classes [11]. Polynomial invariants (under SLOCC) have been used to classify and even quantify the entanglement of multiqubit states [12,13].

For symmetric states, that is, states belonging to the vector space spanned by pure states invariant under particle exchange, the situation is somewhat simpler, in the sense that several entanglement criteria coincide [14]. Continuous sets of SLOCC classes of pure states can be grouped into SLOCC-invariant families based on the degeneracy structure of the involved single particle states [15]. Notably, PPT is equivalent to the positivity of a correlation matrix of moments

of local orthogonal observables [14]. PPT symmetric states of two or three qubits are all separable [16], whereas for four, five, or six qubits entangled symmetric PPT states exist [14,17]. PPT mixed symmetric states for N qubits were studied in [18], where criteria for separability in terms of the ranks of such states were found.

In a parallel line of research, the concept of classical spin states and the notion of quantumness of a spin state was introduced [19–22]. In analogy to quantum optics, a pure spin state is considered (most) classical if the quantum fluctuations of the spin vector are minimal, i.e., as small as allowed by Heisenberg's uncertainty principle. This selects uniquely the SU(2)-coherent states as pure “classical spin states.” Their convex hull is the set of all classical spin states, and the distance of a given state ρ from this convex set is a measure of its “quantumness.” In [20,21] the quantumness based on the Hilbert-Schmidt distance and the Bures distance was analyzed, and the “most quantum” state for these measures identified. Classical states of a spin j are in fact formally identical to fully separable symmetric states of $N = 2j$ spins- $\frac{1}{2}$ (see Sec. II C). Statements about the classicality of spin- j states therefore immediately translate to statements about the separability of symmetric states of multiqubit systems.

In [22], it was noted that PPT for spin-1 states is equivalent to the positivity of a matrix built from tensor entries of a recently introduced tensor representation of the state [23]. The aim of the present work is to generalize this result to arbitrary spin and bipartition. We show that an appropriate arrangement of the components of the tensor representing a spin- j state leads to a matrix that is similar to the partial transposed multiqubit state written in the computational basis. Hence, positivity of this matrix is equivalent to PPT of the multiqubit state. We explicitly construct the unitary transformations that connect the two matrix representations, and show that they generalize the “magic basis” that for two qubits allows one to obtain an explicit form of the concurrence [24]. We also point out the connection to correlation functions that were introduced earlier for studying entanglement of symmetric spin states [14,25,26]. After recalling the basic definitions in Sec. II, we first consider the easier case of an equal bipartition in Sec. III, then move on to the general case in

Sec. IV. In Sec. V we discuss various consequences of our results.

II. CLASSICAL SPIN STATES

A. Tensor representation

Let ρ be a spin- j state (mixed or pure), with j integer or half-integer, and $N = 2j$. In [23] we introduced a tensorial representation of ρ as

$$\rho = \frac{1}{2^N} X_{\mu_1\mu_2\cdots\mu_N} S_{\mu_1\mu_2\cdots\mu_N}, \quad (1)$$

where

$$X_{\mu_1\mu_2\cdots\mu_N} = \text{tr}(\rho S_{\mu_1\mu_2\cdots\mu_N}) \quad (2)$$

is a real symmetric tensor (we use Einstein sum convention, summing over repeated indices). The matrices $S_{\mu_1\mu_2\cdots\mu_N}$ can be obtained from the expansion of the matrix corresponding to the $(j,0)$ representation of a Lorentz boost along a four-vector. Alternately, they can be constructed from Pauli matrices σ^μ , $0 \leq \mu \leq 3$, with σ_0 the 2×2 identity matrix, as the projection of the tensor product $\sigma^{\mu_1} \otimes \sigma^{\mu_2} \otimes \cdots \otimes \sigma^{\mu_N}$ onto the subspace spanned by pure states invariant under permutation [23]. The tensor representation is such that

$$\sum_{a=1}^3 X_{aa\mu_3\cdots\mu_N} = X_{00\mu_3\cdots\mu_N} \quad (3)$$

for arbitrary $0 \leq \mu_3, \dots, \mu_N \leq 3$. The matrix $S_{0\dots 0}$ is the $(N+1) \times (N+1)$ identity matrix, so that in particular, the condition $\text{tr}\rho = 1$ is equivalent to $X_{0\dots 0} = 1$.

B. Classical states

A spin- j coherent state $|\alpha^j\rangle$ associated with the Bloch vector $\mathbf{n} = (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$ is defined as

$$|\alpha^j\rangle = \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(\cos\frac{\theta}{2}\right)^{j+m} \left(\sin\frac{\theta}{2} e^{-i\phi}\right)^{j-m} |j, m\rangle, \quad (4)$$

where $\{|j, m\rangle; -j \leq m \leq j\}$ is the usual angular momentum basis. Such a state has tensor entries given by $X_{\mu_1\mu_2\cdots\mu_N} = n_{\mu_1} n_{\mu_2} \cdots n_{\mu_N}$, with $n = (1, \mathbf{n})$ [23]. For spin- $\frac{1}{2}$ we denote coherent states simply by $|\alpha\rangle$. If $|\alpha^j\rangle$ is written in the N -spins- $\frac{1}{2}$ computational basis, we have the identities

$$|\alpha^j\rangle = |\alpha\rangle \otimes |\alpha\rangle \otimes \cdots \otimes |\alpha\rangle, \quad (5)$$

the tensor product of N copies of the spin- $\frac{1}{2}$ coherent state, and

$$n_\mu = \langle \alpha | \sigma^\mu | \alpha \rangle. \quad (6)$$

In [19] we introduced classical spin states as the convex hull of coherent states, that is, states ρ such that there exists a positive function $P(\alpha)$ defined on the unit sphere and verifying

$$\rho = \int d\alpha P(\alpha) |\alpha^j\rangle \langle \alpha^j|. \quad (7)$$

In tensor terms, classical states are states ρ whose tensor representation is given by

$$X_{\mu_1\mu_2\cdots\mu_N} = \int_{\mathbb{S}} dn P(n) n_{\mu_1} n_{\mu_2} \cdots n_{\mu_N}, \quad (8)$$

where \mathbb{S} is the unit sphere of \mathbb{R}^3 and dn is the flat measure on the sphere. Since we are considering finite-dimensional Hilbert spaces, Caratheodory's theorem ensures that the integral in (8) can be replaced by a finite sum, so that there exist weights $w_i \geq 0$ and vectors $n^{(i)} = (1, \mathbf{n}^{(i)})$ such that

$$X_{\mu_1\mu_2\cdots\mu_N} = \sum_i w_i n_{\mu_1}^{(i)} n_{\mu_2}^{(i)} \cdots n_{\mu_N}^{(i)}. \quad (9)$$

C. Classically and separability

A spin- j state can be seen as the projection of the state of N spins- $\frac{1}{2}$ onto the vector space \mathcal{S} spanned by pure symmetric states. We call a mixed state ρ *symmetric* if it is equal to its projection onto \mathcal{S} . If a convex combination of pure states $\rho = \sum w_i |v_i\rangle \langle v_i|$, with $|v_i\rangle$ pure states and $w_i \geq 0$, is symmetric, then necessarily all $|v_i\rangle$ belong to \mathcal{S} . Indeed, let \mathcal{S}^\perp be the vector space orthogonal to \mathcal{S} . Then for any vector $|u\rangle \in \mathcal{S}^\perp$ the symmetry of ρ implies that $\langle u | \rho | u \rangle = 0$, thus $\sum w_i |\langle u | v_i \rangle|^2 = 0$. Positivity of the w_i then implies that $\langle u | v_i \rangle = 0$, and thus $|v_i\rangle \in (\mathcal{S}^\perp)^\perp = \mathcal{S}$.

Classical spin- j states can thus be seen as separable fully symmetric states of $2j$ spin- $\frac{1}{2}$ states, and vice versa, via the following theorem:

Theorem 1. A symmetric state is (fully) separable if and only if there exists a P representation for which the P function is positive on the two sphere. In other words, classical states are identified with fully separable symmetric states.

This theorem was proved many times in many guises (see, e.g., [27], p. 4 or [28]). For completeness we briefly give a proof of this fact.

Proof. If ρ is fully separable, then it is possible to write $\rho = \sum_i \lambda_i \rho_1^{(i)} \otimes \cdots \otimes \rho_N^{(i)}$, and then to decompose each $\rho_k^{(i)}$ in its eigenvector basis, so that

$$\begin{aligned} \rho &= \sum_i \mu_i |v_1^{(i)}\rangle \langle v_1^{(i)}| \otimes \cdots \otimes |v_N^{(i)}\rangle \langle v_N^{(i)}| \\ &= \sum_i \mu_i |v_1^{(i)} \cdots v_N^{(i)}\rangle \langle v_1^{(i)} \cdots v_N^{(i)}|, \end{aligned} \quad (10)$$

with $\mu_i \geq 0$. Since ρ is symmetric one has $|v_1^{(i)} \cdots v_N^{(i)}\rangle \in \mathcal{S}$. The symmetry imposes that $|v_1^{(i)}\rangle = \cdots = |v_N^{(i)}\rangle$. As spin- $\frac{1}{2}$ states are all coherent states and from Eq. (5) the tensor product of identical spin- $\frac{1}{2}$ coherent states yields a spin- j coherent state, this completes the proof. The converse is obvious, since inserting (5) into (7) shows that any classical state is separable and symmetric. ■

Seeing a spin- j state as a multipartite state allows one to define partial operations on subsystems, such as partial tracing or partial transposition. An important property of the tensor representation (1) is the following: the partial trace of a state ρ with tensor $X_{\mu_1\mu_2\cdots\mu_N}$, taken over $N - k$ qubits, is a symmetric k -qubit state with tensor coefficients $X_{\mu_1\cdots\mu_k 0\dots 0}$ [23]. This will allow us to reexpress various separability criteria in terms of the $X_{\mu_1\mu_2\cdots\mu_N}$.

D. Separability criteria

Using the correspondence outlined above, classicality criteria can be obtained from known separability criteria, such as the PPT criterion. Let us consider a bipartite quantum state $\rho \in \mathcal{H}_1 \otimes \mathcal{H}_2$, with $\mathcal{H}_1, \mathcal{H}_2$ two finite-dimensional Hilbert spaces of dimension d_1 and d_2 , respectively. The partial transpose of ρ with respect to subsystem 2 is defined by

$$(\rho^{\text{PT}})_{i_1 i_2, j_1 j_2} = \rho_{i_1 j_2, j_1 i_2}, \quad 0 \leq i_k, j_k \leq d_k - 1. \quad (11)$$

Peres [4] showed that positivity of the partial transpose matrix ρ^{PT} is a necessary condition for separability. It was conjectured [4] and later proved [5] that PPT is a necessary and sufficient condition in the case where $d_A = 2$ and $d_B = 2$ or 3.

In the case of classical spin- j states seen as fully separable symmetric states of $N = 2j$ spins- $\frac{1}{2}$, PPT yields a necessary criterion for any bipartition of the N qubits into r and $N - r$ qubits. As the state is symmetric this criterion only depends on the number r of the qubits and not on which qubits are chosen. We denote by $\text{PT}(N - r : r)$ the partial transpose matrix associated with such a bipartition, where transposition only affects the Hilbert space associated with the last r qubits. For instance, for a five-qubit separable state $\rho_1 \otimes \rho_2 \otimes \rho_3 \otimes \rho_4 \otimes \rho_5$ we have $\text{PT}(3 : 2) = \rho_1 \otimes \rho_2 \otimes \rho_3 \otimes \rho_4^T \otimes \rho_5^T$. As $\text{PT}(r : N - r)$ is the transpose of the matrix $\text{PT}(N - r : r)$ we shall only consider the case $r \leq j$.

The Peres separability criterion [4] gives as a necessary classicality criterion

$$\text{PT}(N - r : r) \geq 0, \quad 1 \leq r \leq N/2. \quad (12)$$

For states of two or three qubits, the Peres-Horodecki criterion [5] yields a necessary and sufficient separability condition that reads

$$\text{PT}(N - 1 : 1) \geq 0. \quad (13)$$

Equivalently, with $j = N/2$, this gives a necessary and sufficient classicality condition for spin- j states with $j = 1$ or $j = 3/2$.

III. PPT AND TENSOR REPRESENTATION

A. Matrix T for equal bipartition

In this section we reformulate the classicality criterion (12) for integer j and equal bipartition ($j : j$) in terms of tensor entries $X_{\mu_1 \mu_2 \dots \mu_N}$. We start by introducing the $4^j \times 4^j$ matrix

$$T_{\mu, \nu} = X_{\mu_1 \dots \mu_j \nu_1 \dots \nu_j}, \quad (14)$$

where matrix indices are vectors $\mu = (\mu_1 \dots \mu_j)$ and $\nu = (\nu_1 \dots \nu_j)$, $0 \leq \mu_i, \nu_i \leq 3$. [In this paper we use commas to separate the two (multi-)indices of a square matrix, while tensor indices have no commas.] According to the definition of $X_{\mu_1 \dots \mu_N}$, the matrix elements of T can all be obtained as expectation values of tensor products of Pauli operators. The matrix T is real and symmetric. It turns out, as we will show, that $\rho^{\text{PT}} = \text{PT}(j : j)$ is similar to a multiple of T , that is, there exists a unitary matrix R and a (positive) constant λ such that $R^\dagger \rho^{\text{PT}} R = \lambda T$. In particular, this implies that for the equal bipartition ($j : j$), the positivity of the partial transpose ρ^{PT} is equivalent to the positivity of the matrix T , so that the corresponding necessary classicality criterion can

be expressed as $T \geq 0$. We first examine the cases of small j and then move on to the general situation.

B. Spin-1 case

In the spin-1 case the matrix T in (14) coincides with the 4×4 matrix X , since the multi-indices μ and ν reduce to single indices μ and ν , $0 \leq \mu, \nu \leq 3$. Let ρ^{PT} be the partial transpose of the spin-1 state ρ written in the canonical basis of two qubits; it can be expressed as in (11). We want to find a 4×4 unitary matrix R with the property that

$$(R^\dagger)_{\mu, i_1 i_2} \rho_{i_1 j_2, j_1 i_2} R_{j_1 j_2, \nu} = \lambda X_{\mu, \nu} \quad (15)$$

with $0 \leq i_1, i_2, j_1, j_2 \leq 1$ and $0 \leq \mu, \nu \leq 3$. Suppose that ρ is a coherent state. Then the left-hand side of Eq. (15) reads

$$(R^\dagger)_{\mu, i_1 i_2} (|\alpha\rangle\langle\alpha|)_{i_1, j_1} (|\alpha\rangle\langle\alpha|)_{j_2, i_2} R_{j_1 j_2, \nu}, \quad (16)$$

which can be rewritten as

$$\langle\alpha|_{i_2} (R^\dagger)_{\mu, i_1 i_2} |\alpha\rangle_{i_1} \langle\alpha|_{j_1} R_{j_1 j_2, \nu} |\alpha\rangle_{j_2}, \quad (17)$$

while from Eq. (6) the tensor coordinates of ρ can be expressed as $X_{\mu, \nu} = \langle\alpha|\sigma^\mu|\alpha\rangle\langle\alpha|\sigma^\nu|\alpha\rangle$. One easily checks that a possible choice of R that complies with Eq. (15) is

$$R_{i_1 i_2, \mu} = \frac{1}{\sqrt{2}} \sigma_{i_1, i_2}^\mu \quad (18)$$

together with $\lambda = 1/2$. Since R and λ chosen are both independent of $|\alpha\rangle$, they will in fact fulfill Eq. (15) for any coherent state. As any density matrix ρ can be expanded as a linear combination of coherent states [as in (7), but possibly with a negative P function], R and λ will be suited for any density matrix. Moreover, the matrix R is unitary since

$$(R^\dagger R)_{\mu, \nu} = \frac{1}{2} \text{tr}\{\sigma^\mu \sigma^\nu\} = \delta_{\mu, \nu}, \quad (19)$$

with $\delta_{\mu, \nu}$ the Kronecker symbol. Thus, $(R^\dagger \rho^{\text{PT}} R)_{\mu, \nu} = \lambda X_{\mu, \nu}$, so that the PPT criterion $\text{PT}(1 : 1) \geq 0$ is equivalent to positivity of the 4×4 matrix $(X_{\mu, \nu})_{0 \leq \mu, \nu \leq 3}$.

C. Spin-2 case

For spin 2, the matrix T is indexed by multi-indices $(\mu_1 \mu_2)$ and $(\nu_1 \nu_2)$, while the matrix ρ expressed in the computational basis of qubits is indexed by multi-indices $(i_1 i_2 i_3 i_4)$ and $(j_1 j_2 j_3 j_4)$, with again $i_k, j_k \in \{0, 1\}$ and $\mu_k, \nu_k \in \{0, 1, 2, 3\}$. We are looking for a unitary matrix R and a constant λ such that $R^\dagger \rho^{\text{PT}} R = \lambda T$, with ρ^{PT} the partial transpose taken over the last two qubits. As before, we can first consider the case where ρ is a coherent state. Explicitly, the analog of Eq. (16) for the components of $R^\dagger \rho^{\text{PT}} R$ reads

$$(R^\dagger)_{\mu_1 \mu_2, i_1 i_2 i_3 i_4} |\alpha\rangle\langle\alpha|_{i_1, j_1} |\alpha\rangle\langle\alpha|_{i_2, j_2} \times |\alpha\rangle\langle\alpha|_{j_3, i_3} |\alpha\rangle\langle\alpha|_{j_4, i_4} R_{j_1 j_2 j_3 j_4, \nu_1 \nu_2}, \quad (20)$$

while the analog of (17) reads

$$\langle\alpha|_{i_3} \langle\alpha|_{i_4} (R^\dagger)_{\mu_1 \mu_2, i_1 i_2 i_3 i_4} |\alpha\rangle_{i_1} |\alpha\rangle_{i_2} \times \langle\alpha|_{j_1} \langle\alpha|_{j_2} R_{j_1 j_2 j_3 j_4, \nu_1 \nu_2} |\alpha\rangle_{j_3} |\alpha\rangle_{j_4}. \quad (21)$$

The matrix T can now be written as

$$\langle\alpha|\sigma^{\mu_1}|\alpha\rangle\langle\alpha|\sigma^{\mu_2}|\alpha\rangle\langle\alpha|\sigma^{\nu_1}|\alpha\rangle\langle\alpha|\sigma^{\nu_2}|\alpha\rangle. \quad (22)$$

A choice of R and λ that fulfills the required relation between (21) and (22) is

$$R_{i_1 i_2 i_3 i_4, \mu_1 \mu_2} = \frac{1}{2} \sigma_{i_1, i_3}^{\mu_1} \sigma_{i_2, i_4}^{\mu_2}. \quad (23)$$

The corresponding value of λ is then $\lambda = 1/4$. Note that other choices are possible for R : a different solution would be $\frac{1}{2} \sigma_{i_1, i_4}^{\mu_1} \sigma_{i_2, i_3}^{\mu_2}$. Since R and λ are independent of $|\alpha\rangle$, they are valid for any coherent state and thus for any density matrix ρ . Unitarity of the matrix R comes from the identity

$$(R^\dagger R)_{\mu, \nu} = \frac{1}{4} \text{tr}\{\sigma^{\mu_1} \sigma^{\nu_1}\} \text{tr}\{\sigma^{\mu_2} \sigma^{\nu_2}\} = \delta_{\mu_1 \nu_1} \delta_{\mu_2 \nu_2}, \quad (24)$$

with $\boldsymbol{\mu} = (\mu_1 \mu_2)$, $\boldsymbol{\nu} = (\nu_1 \nu_2)$. Therefore, the necessary PPT criterion (12) for spin-2 states can be expressed as $T \geq 0$, where T is the 16×16 matrix defined by $T_{\boldsymbol{\mu}, \boldsymbol{\nu}} = X_{\mu_1 \mu_2 \nu_1 \nu_2}$.

D. General case

The above construction easily generalizes to higher integer spin sizes. For spin j the $4^j \times 4^j$ matrix R reads

$$R_{\mathbf{i}, \boldsymbol{\mu}} = \frac{1}{2^{j/2}} \prod_{k=1}^j \sigma_{i_k, i_{k+j}}^{\mu_k}, \quad (25)$$

where $\mathbf{i} = (i_1 i_2 \dots i_N)$ and $\boldsymbol{\mu} = (\mu_1 \mu_2 \dots \mu_j)$, with $0 \leq \mu_k \leq 3$ and $0 \leq i_k \leq 1$. Note that each Pauli matrix is indexed by one index associated with a nontransposed qubit and one associated with a transposed qubit. Any such pairing would yield a valid R . It is easy to check that matrices R are unitary and such that $R^\dagger \rho^{\text{PT}} R = \lambda T$, with $\rho^{\text{PT}} = \text{PT}(j : j)$ and $\lambda = 1/2^j$. Thus, the corresponding PPT criterion yields the classicality criterion $T \geq 0$.

IV. PPT FOR ANY BIPARTITION

A. $T^{(r)}$ matrices

The results of Sec. III can be further generalized to uneven bipartitions of symmetric states. In this section we show that matrices $\text{PT}(N - r : r)$ are similar to a multiple of matrices $T^{(r)}$ defined by

$$T_{\boldsymbol{\mu}, \mathbf{i}, \boldsymbol{\nu}}^{(r)} = X_{\tau_1 \dots \tau_{N-2r}, \mu_1 \dots \mu_r, \nu_1 \dots \nu_r} \prod_{k=1}^{N-2r} \sigma_{i_k, i'_k}^{\tau_k}, \quad (26)$$

where $\boldsymbol{\mu} = (\mu_1 \dots \mu_r)$, $\boldsymbol{\nu} = (\nu_1 \dots \nu_r)$, $\mathbf{i} = (i_1 \dots i_{N-2r})$, and $\mathbf{i}' = (i'_1 \dots i'_{N-2r})$ are multi-indices with $0 \leq \mu_k \leq 3$ and $0 \leq i_k, i'_k \leq 1$, and summation over the $\tau_k \in \{0, 1, 2, 3\}$ is implicit. In this definition, indices $\boldsymbol{\nu}$ are associated with the transposed subspace, while indices $\boldsymbol{\tau}$ and $\boldsymbol{\mu}$ are associated with the nontransposed one. Matrices $T^{(r)}$ are of size $4^j \times 4^j$. In the case of equal bipartition $r = j$, Eq. (26) reduces to Eq. (14).

B. Spin 3/2

Let us start by considering the smallest-size case. Let ρ be a spin-3/2 state and $\rho^{\text{PT}} = \text{PT}(2 : 1)$, its transpose with respect to the third qubit. The matrix $T^{(1)}$ in Eq. (26) is given by

$$T_{\boldsymbol{\mu}, \mathbf{i}, \boldsymbol{\nu}}^{(1)} = X_{\tau \mu \nu} \sigma_{i, i'}^{\tau}. \quad (27)$$

Building on the results of the previous section, it is easy to construct a unitary matrix R such that $R^\dagger \rho^{\text{PT}} R = \lambda T^{(r)}$. As

before we consider the case where ρ is a coherent state. In such a case, $R^\dagger \rho^{\text{PT}} R$ reduces to

$$(R^\dagger)_{\boldsymbol{\mu}, \mathbf{i}, a_1 a_2 a_3} |\alpha\rangle \langle \alpha|_{a_1, b_1} \times |\alpha\rangle \langle \alpha|_{a_2, b_2} |\alpha\rangle \langle \alpha|_{b_3, a_3} R_{b_1 b_2 b_3, \boldsymbol{\nu}, i'}, \quad (28)$$

with $0 \leq a_k, b_k \leq 1$, or equivalently

$$\langle \alpha|_{a_3} (R^\dagger)_{\boldsymbol{\mu}, \mathbf{i}, a_1 a_2 a_3} |\alpha\rangle_{a_1} |\alpha\rangle_{a_2} \langle \alpha|_{b_1} \langle \alpha|_{b_2} R_{b_1 b_2 b_3, \boldsymbol{\nu}, i'} |\alpha\rangle_{b_3}, \quad (29)$$

while the matrix $T^{(1)}$ defined in (27) can be written for this coherent state $|\alpha\rangle$ as

$$\langle \alpha| \sigma^\mu |\alpha\rangle \langle \alpha| \sigma^\nu |\alpha\rangle \langle 2|\alpha\rangle \langle \alpha|_{i, i'} \quad (30)$$

(we used the fact that $\frac{1}{2} n_\tau \sigma^\tau = |\alpha\rangle \langle \alpha|$). Identifying Eqs. (29) and (30) up to a constant we see that a unitary R can be defined, for instance, as

$$R_{a_1 a_2 a_3, \boldsymbol{\mu}, \mathbf{i}} = \frac{1}{\sqrt{2}} \delta_{a_1, i} \sigma_{a_2, a_3}^{\boldsymbol{\mu}}. \quad (31)$$

In fact, the indices a_2, a_3 of the matrix σ^μ in (31) have to pair any index associated with the nontransposed subspace with an index associated with the transposed subspace, while the delta function pairs the remaining indices in (29), leading to the projector $|\alpha\rangle \langle \alpha|$ in (30). Unitarity of R is easily verified, since

$$(R^\dagger R)_{\boldsymbol{\mu}, \mathbf{i}, \boldsymbol{\nu}, i'} = \frac{1}{2} \text{tr}\{\sigma^\mu \sigma^\nu\} \sum_{i_2} \delta_{i_1, i_2} \delta_{i_2, i'} = \delta_{\boldsymbol{\mu}, \boldsymbol{\nu}} \delta_{i, i'}. \quad (32)$$

As in the equal bipartition case, linearity ensures that R defined in (31) together with $\lambda = 1/4$ is such that $R^\dagger \rho^{\text{PT}} R = \lambda T^{(r)}$.

C. General R matrices

The above case contains the essence of the general proof and generalizes to arbitrary values of j and r . In order to recover matrix $T^{(r)}$ from $\text{PT}(N - r : r)$, we have to construct a matrix R built out of products of σ^μ matrices and Kronecker deltas, such that the Pauli matrices pair r indices among those associated with the nontransposed subspace together with all r indices associated with the transposed subspace. The remaining $N - 2r$ indices, corresponding to the remaining part of the nontransposed subspace, go into Kronecker deltas. More precisely, we choose these latter indices to be the $N - 2r$ first ones, and to pair indices k with $k + r$ for $N - 2r + 1 \leq k \leq N - r$. We thus define matrices $R^{(r)}$ by

$$R_{\mathbf{a}, \boldsymbol{\mu}, \mathbf{i}}^{(r)} = \frac{1}{2^{r/2}} \prod_{k=1}^{N-2r} \delta_{a_k, i_k} \prod_{k=1}^r \sigma_{a_{N-2r+k}, a_{N-r+k}}^{\mu_k}, \quad (33)$$

with $\mathbf{a} = (a_1 \dots a_N)$, $\boldsymbol{\mu} = (\mu_1 \dots \mu_r)$, and $\mathbf{i} = (i_1 \dots i_{N-2r})$, with $\mu_k \in \{0, 1, 2, 3\}$ and $a_k, i_k \in \{0, 1\}$. One can check, as above, that $R^{(r)}$ are unitary and such that

$$(R^{(r)})^\dagger \rho^{\text{PT}} R^{(r)} = \frac{1}{2^{N-r}} T^{(r)} \quad (34)$$

with $\rho^{\text{PT}} = \text{PT}(N - r : r)$. Unitarity trivially comes from the fact that indices of the Pauli matrices and the Kronecker deltas in (33) are all distinct, so that the identity (19) can be applied to each pair of matrices. To show (34), we first write ρ^{PT} in the computational basis with the help of the tensor representation. As explained in Sec. II, the expansion (1) can

be obtained by projecting tensor products of Pauli matrices onto the symmetric subspace. In the computational basis of N qubits, ρ can thus be expressed as

$$\rho = \frac{1}{2^N} X_{\mu_1 \mu_2 \dots \mu_N} \sigma^{\mu_1} \otimes \sigma^{\mu_2} \otimes \dots \otimes \sigma^{\mu_N}, \quad (35)$$

so that ρ^{PT} reads

$$\rho_{\mathbf{a}, \mathbf{b}}^{\text{PT}} = \frac{1}{2^N} X_{\tau_1 \dots \tau_N} \prod_{k=1}^{N-r} \sigma_{a_k, b_k}^{\tau_k} \prod_{k=N-r+1}^N \sigma_{b_k, a_k}^{\tau_k} \quad (36)$$

with $\mathbf{a} = (a_1 \dots a_N)$ and $\mathbf{b} = (b_1 \dots b_N)$, $a_k, b_k \in \{0, 1\}$. The left-hand side of (34) has components

$$[(R^{(r)})^\dagger \rho^{\text{PT}} R^{(r)}]_{\mu, \mathbf{i}, \nu, \mathbf{i}'} = (R_{\mathbf{a}, \mu, \mathbf{i}}^{(r)})^* \rho_{\mathbf{a}, \mathbf{b}}^{\text{PT}} R_{\mathbf{b}, \nu, \mathbf{i}'}, \quad (37)$$

where $*$ denotes complex conjugation. Using (33) and (36), this can be expressed as

$$\begin{aligned} & \frac{1}{2^{r+N}} X_{\tau_1 \dots \tau_N} \prod_{k=1}^{N-2r} \delta_{a_k, i_k} \prod_{k=N-2r+1}^{N-r} \sigma_{a_{k+r}, a_k}^{\mu_{k-N+2r}} \prod_{k=1}^{N-r} \sigma_{b_k, b_{k+r}}^{\tau_k} \\ & \times \prod_{k=N-r+1}^N \sigma_{b_k, a_k}^{\tau_k} \prod_{k=1}^{N-2r} \delta_{b_k, i'_k} \prod_{k=N-2r+1}^{N-r} \sigma_{b_k, b_{k+r}}^{\nu_{k-N+2r}}. \end{aligned} \quad (38)$$

The above product contains terms

$$\delta_{a_k, i_k} \sigma_{a_k, b_k}^{\tau_k} \delta_{b_k, i'_k} = \sigma_{i_k, i'_k}^{\tau_k} \quad (39)$$

for $1 \leq k \leq N - 2r$, terms

$$\sigma_{a_{k+r}, a_k}^{\mu_{k-N+2r}} \sigma_{a_k, b_k}^{\tau_k} \sigma_{b_k, b_{k+r}}^{\nu_{k-N+2r}} = (\sigma^{\mu_{k-N+2r}} \sigma^{\tau_k} \sigma^{\nu_{k-N+2r}})_{a_{k+r}, b_{k+r}} \quad (40)$$

for $N - 2r + 1 \leq k \leq N - r$, and terms

$$\sigma_{b_k, a_k}^{\tau_k} \quad (41)$$

for $N - r + 1 \leq k \leq N$ (recall that we are considering a case where $N - r \geq r$). Taking the product of all terms (39)–(41)

and summing over the remaining a_k and b_k (those with $N - r + 1 \leq k \leq N$), (38) becomes

$$\frac{X_{\tau_1 \dots \tau_N}}{2^{r+N}} \prod_{k=1}^{N-2r} \sigma_{i_k, i'_k}^{\tau_k} \prod_{k=1}^r \text{tr}\{\sigma^{\mu_k} \sigma^{\tau_{k+N-2r}} \sigma^{\nu_k} \sigma^{\tau_{k+N-r}}\}. \quad (42)$$

As can be checked explicitly, one has the identity

$$\frac{1}{4} y_{\tau, \tau'} \text{tr}\{\sigma^\mu \sigma^\tau \sigma^\nu \sigma^{\tau'}\} = y_{\mu, \nu} \quad (43)$$

for any real symmetric matrix $(y_{\mu, \nu})_{0 \leq \mu, \nu \leq 3}$ such that $\sum_{a=1}^3 y_{aa} = y_{00}$. Applying this identity to the summation over pairs of indices $(\tau_{k+N-2r}, \tau_{k+N-r})$ for $1 \leq k \leq r$ in (42) [and using property (3) of the tensor], we recover the term $X_{\tau_1 \dots \tau_{N-2r}, \mu_1 \dots \mu_r, \nu_1 \dots \nu_r}$ of (26). The product of terms (39) yields the Pauli matrix terms in (26). The overall remaining factor is $\lambda = 1/2^{N-r}$. This proves Eq. (34).

V. SOME CONSEQUENCES

A. PPT criteria

As mentioned in Sec. IID, the PPT separability criterion provides necessary, and in some instances sufficient, classicality criteria. The previous sections have shown that the partial transpose takes a very simple form for symmetric states expressed as in (1). Thus each PPT criterion is equivalent to a linear matrix inequality $T^{(r)} \geq 0$. In the simplest case of spin-1 states, $T^{(r)}$ is given by Eq. (14), so that the PPT criterion $\text{PT}(1:1) \geq 0$ is equivalent to $X \geq 0$ for the 4×4 matrix $(X_{\mu, \nu})_{0 \leq \mu, \nu \leq 3}$. This was already observed in [22], where the same relation between ρ^{PT} and X was obtained. Our present results generalize this relation: For integer spin and equal bipartition $r = j$, the $\text{PT}(j:j)$ criterion is expressed in a very transparent way in our tensor language, as the positivity of the matrix $(T_{\mu, \nu})$ indexed by j tuples of indices and defined in (14). More generally, each PPT criterion yields a classicality criterion as the positivity of a matrix $T^{(r)}$.

In the case of spin- $\frac{3}{2}$, using the results of Sec. IV, a necessary and sufficient classicality criterion can be expressed as $T^{(1)} \geq 0$, where $T^{(1)}$ is defined in (27). In terms of the tensor entries, this criterion reads

$$\begin{pmatrix} X_{000} + X_{003} & X_{001} - iX_{002} & X_{001} + X_{013} & X_{011} - iX_{012} & X_{002} + X_{023} & X_{012} - iX_{022} & X_{003} + X_{033} & X_{013} - iX_{023} \\ X_{001} + iX_{002} & X_{000} - X_{003} & X_{011} + iX_{012} & X_{001} - X_{013} & X_{012} + iX_{022} & X_{002} - X_{023} & X_{013} + iX_{023} & X_{003} - X_{033} \\ X_{001} + X_{013} & X_{011} - iX_{012} & X_{011} + X_{113} & X_{111} - iX_{112} & X_{012} + X_{123} & X_{112} - iX_{122} & X_{013} + X_{133} & X_{113} - iX_{123} \\ X_{011} + iX_{012} & X_{001} - X_{013} & X_{111} + iX_{112} & X_{011} - X_{113} & X_{112} + iX_{122} & X_{012} - X_{123} & X_{113} + iX_{123} & X_{013} - X_{133} \\ X_{002} + X_{023} & X_{012} - iX_{022} & X_{012} + X_{123} & X_{112} - iX_{122} & X_{022} + X_{223} & X_{122} - iX_{222} & X_{023} + X_{233} & X_{123} - iX_{223} \\ X_{012} + iX_{022} & X_{002} - X_{023} & X_{112} + iX_{122} & X_{012} - X_{123} & X_{122} + iX_{222} & X_{022} - X_{223} & X_{123} + iX_{223} & X_{023} - X_{233} \\ X_{003} + X_{033} & X_{013} - iX_{023} & X_{013} + X_{133} & X_{113} - iX_{123} & X_{023} + X_{233} & X_{123} - iX_{223} & X_{033} + X_{333} & X_{133} - iX_{233} \\ X_{013} + iX_{023} & X_{003} - X_{033} & X_{113} + iX_{123} & X_{013} - X_{133} & X_{123} + iX_{223} & X_{023} - X_{233} & X_{133} + iX_{233} & X_{033} - X_{333} \end{pmatrix} \geq 0. \quad (44)$$

This matrix inequality can in turn be expressed as positivity of a 16×16 real symmetric matrix, whose entries are of the form $\pm X_{\mu_1 \mu_2 \mu_3}$, i.e., $\pm(\sigma^{\mu_1} \otimes \sigma^{\mu_2} \otimes \sigma^{\mu_3})$, which provides a necessary and sufficient classicality condition as positivity of a matrix of observables.

B. Correlation matrices

Let X be the tensor representation (2) of a spin- j state ρ with j integer. We define correlation matrices associated with the tensor X as the $4^r \times 4^r$ matrices ($1 \leq r \leq j$)

$$C_{\mu_r, \nu_r}^{(r)} = X_{\mu_r, \nu_r, \mathbf{0}_{N-2r}} - X_{\mu_r, \mathbf{0}_{N-r}} X_{\nu_r, \mathbf{0}_{N-r}}, \quad (45)$$

where $\boldsymbol{\mu}_r = (\mu_1 \cdots \mu_r)$, $\mathbf{v}_r = (v_1 \cdots v_r)$, and $\mathbf{0}_k$ is the zero vector of length k . Since the first line and column of $C^{(r)}$ are indexed by $\mathbf{0}_r$, and $X_{0 \dots 0} = 1$, it takes the form

$$C^{(r)} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & S^{(r)} & \\ 0 & & & \end{pmatrix}, \quad (46)$$

where the matrix $S^{(r)}$ is of size $(4^r - 1) \times (4^r - 1)$. In terms of the entries of the matrix T defined in (14), $S^{(r)}$ can be expressed as

$$S_{\boldsymbol{\mu}_r, \mathbf{v}_r}^{(r)} = T_{\boldsymbol{\mu}_r, \mathbf{0}_{j-r}, \mathbf{v}_r, \mathbf{0}_{j-r}} - T_{\boldsymbol{\mu}_r, \mathbf{0}_{j-r}, \mathbf{0}_j} T_{\mathbf{v}_r, \mathbf{0}_{j-r}, \mathbf{0}_j}. \quad (47)$$

The matrix $S^{(r)}$ can thus be interpreted as the Schur complement of the matrix $(T_{\boldsymbol{\mu}_r, \mathbf{0}_{j-r}, \mathbf{v}_r, \mathbf{0}_{j-r}})_{\boldsymbol{\mu}_r, \mathbf{v}_r}$ with respect to the upper left entry $T_{\mathbf{0}_j, \mathbf{0}_j} = 1$. The matrix $(T_{\boldsymbol{\mu}_r, \mathbf{0}_{j-r}, \mathbf{v}_r, \mathbf{0}_{j-r}})_{\boldsymbol{\mu}_r, \mathbf{v}_r}$ is the restriction of T to its 4^r first lines and columns. This $4^r \times 4^r$ subblock coincides with the matrix T associated with the spin- r state ρ_r obtained from ρ by tracing over $N - 2r$ qubits. Since positivity of a matrix is equivalent to positivity of its Schur complement (if the part complemented is itself positive), one has that the upper left $4^r \times 4^r$ block of T is positive if and only if $C^{(r)} \geq 0$. Together with the results of the previous sections, this shows that the PPT criterion $\text{PT}(j : j) \geq 0$ applied to ρ is equivalent to positivity of the correlation matrix $C^{(j)}$, and more generally the PPT criterion $\text{PT}(r : r) \geq 0$ applied to the reduced density matrix ρ_r is equivalent to positivity of the correlation matrix $C^{(r)}$.

If ρ is a classical state, then all its reduced density matrices ρ_r are classical as well. The PPT criterion thus leads to a sequence of necessary classicality conditions $C^{(r)} \geq 0$. These conditions are those obtained by different means in [25], where the so-called ‘‘intergroup covariance matrices’’ coincide with our matrices $C^{(r)}$. This also allows us to recover results from [14] that the partial transpose criterion for partition into two equally sized subsystems is equivalent to positivity of the correlation matrix of local orthogonal observables.

From the above considerations, we see that all these necessary conditions are encompassed in a compact way in the single condition $T \geq 0$. This latter condition is not sufficient, nor is the condition that all partial transposes be positive. For instance, there exist symmetric four-qubit entangled states for which all partial transposes are positive [17].

C. Teleportation and generalized magic bases

The matrix $R_{\mathbf{i}, \boldsymbol{\mu}} = \frac{1}{\sqrt{2}} \sigma_{i_1, i_2}^{\boldsymbol{\mu}}$ with $\mathbf{i} = (i_1, i_2)$ defined in (18) can be written out explicitly in the computational basis as

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -i & 0 \\ 0 & 1 & i & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix}. \quad (48)$$

The $\boldsymbol{\mu}$ th column of R contains the elements of the Pauli matrix $\sigma^{\boldsymbol{\mu}}$ (up to normalization). These are equal, up to a phase factor, to the two-qubit Bell states. More precisely, the Bell states are the columns of the matrix $\tilde{R}_{i_1 i_2, \boldsymbol{\mu}} = \frac{1}{\sqrt{2}} \tilde{\sigma}_{i_1, i_2}^{\boldsymbol{\mu}}$, where

$\tilde{\sigma}^{\boldsymbol{\mu}} = \sigma^{\boldsymbol{\mu}}$ for $\boldsymbol{\mu} \neq 2$ and $\tilde{\sigma}^{\boldsymbol{\mu}} = i\sigma^{\boldsymbol{\mu}}$ for $\boldsymbol{\mu} = 2$. They are also proportional to the magic basis introduced in [29]: namely, the three last columns of R have to be multiplied by $-i$ in order to recover the magic basis of [29]. We recall that, among other properties, the magic basis is such that when a state $|\psi\rangle$ is written in this basis, with some coefficients α_i , $1 \leq i \leq 4$, then its concurrence is given by $C(|\psi\rangle) = |\sum_{i=1}^4 \alpha_i^2|$.

Bell states are used in the quantum teleportation protocol of a single qubit [2]. If Alice and Bob share a Bell state, it is possible for them to teleport a one-qubit state by exchanging only two classical bits. In a similar spirit, four-qubit generalized Bell states $|g_i\rangle$, $1 \leq i \leq 16$, were introduced in [30]: if Alice and Bob share one of these generalized Bell states, they are able to teleport a two-qubit pure state by exchanging four classical bits (the protocol of [30] is essentially the same as in the one-qubit case). It turns out that the columns of our spin-2 matrix R , defined explicitly in (23), are equal, up to a phase factor, to the 16 states $|g_i\rangle$. More precisely, the $|g_i\rangle$ of [30] are exactly the columns of the matrix

$$\tilde{R}_{i_1 i_2 i_3 i_4, \boldsymbol{\mu}_1 \boldsymbol{\mu}_2} = \frac{1}{2} \tilde{\sigma}_{i_1, i_3}^{\boldsymbol{\mu}_1} \tilde{\sigma}_{i_2, i_4}^{\boldsymbol{\mu}_2} \quad (49)$$

(again the $\tilde{\sigma}$ are such that $\tilde{\sigma}^{\boldsymbol{\mu}} = i\sigma^{\boldsymbol{\mu}}$ for $\boldsymbol{\mu} = 2$, and $\sigma^{\boldsymbol{\mu}}$ otherwise). The generalized Bell basis also provides a generalization of the magic basis to higher qubits. The two-qubit magic basis $|e_i\rangle$, $1 \leq i \leq 16$, in [30] is constructed by multiplying the $|g_i\rangle$ by appropriate phases. A state expressed in this basis as $|\psi\rangle = \sum_{i=1}^{16} \alpha_i |e_i\rangle$ is then such that the generalized concurrence [31] is given by $C(|\psi\rangle) = |\sum_{i=1}^{16} \alpha_i^2|$. We can recover the magic basis $|e_i\rangle$ just by multiplying by i the eight columns of \tilde{R} indexed by pairs $(\boldsymbol{\mu}_1, \boldsymbol{\mu}_2)$ such that $|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2| = 1$. Our formula thus provides a very compact form both for the Bell states appearing in the two-qubit teleportation protocol and for the generalized magic basis of [30].

It is clear from Eq. (49), and from the general form (25) of matrices R , that this approach can be straightforwardly generalized to an arbitrary number of qubits. The N -qubit teleportation protocol proposed in [30] was obtained from the action of products of the form $(\sigma^z)^\alpha (\sigma^x)^\beta$, with $\alpha, \beta \in \{0, 1\}$, on a state $\sum_{j=0}^{N-1} |j\rangle |j\rangle$. Using the fact that $\sigma^z \sigma^x = i\sigma^y$, one can check that the generalized Bell basis coincides, up to phases, with the columns of our matrices. In particular, this means that R can also be interpreted as the unitary matrix that Alice has to apply on her side to make a Bell measurement in the N -qubit teleportation protocol.

VI. CONCLUSION

The present results provide a unifying framework for various concepts dealing with symmetric states. It allows us to reformulate several known results in a much simpler way. In the language of the tensor representation, criteria such as the PPT separability criterion can be expressed in a much more transparent way by positivity of the matrix T . In particular, this allows one to directly relate the partial transpose to correlations of observables, which provides a physical interpretation of the partial transpose beyond time reversal. Note that the matrix R in (48) was used in [32] to generate local unitary invariants in terms of partial transpose and realignments. It may be possible to extend our expressions to that setting as well.

Furthermore, such representations may also be generalized to qudit symmetric states, that is, symmetric tensor products of d -level systems. However, the symmetric sectors are then less easy to describe and their description would require additional work.

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A.3. Tensor eigenvalues and entanglement of symmetric states

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Tensor eigenvalues and entanglement of symmetric states

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Tensor eigenvalues and eigenvectors have been introduced in the recent mathematical literature as a generalization of the usual matrix eigenvalues and eigenvectors. We apply this formalism to a tensor that describes a multipartite symmetric state or a spin state, and we investigate to what extent the corresponding tensor eigenvalues contain information about the multipartite entanglement (or, equivalently, the quantumness) of the state. This extends previous results connecting entanglement to spectral properties related to the state. We show that if the smallest tensor eigenvalue is negative, the state is detected as entangled. While for spin-1 states the positivity of the smallest tensor eigenvalue is equivalent to separability, we show that for higher values of the angular momentum there is a correlation between entanglement and the value of the smallest tensor eigenvalue.

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I. INTRODUCTION

In the study of multipartite entanglement, symmetric multipartite states have drawn some attention recently [1–3]. One reason for that is that they span a Hilbert space whose dimension grows only linearly with the number of constituents, rather than exponentially for arbitrary multipartite states. They are therefore easier to deal with than generic states, and they provide a first step towards a more general understanding of multipartite entanglement. A pure symmetric N -qubit state can be written as a superposition of the Dicke states familiar in quantum optics. A Dicke state is a state of N two-level atoms (i.e., qubits) where a given number of excitations is symmetrically distributed over the N constituents, so that the state is invariant under permutations of the qubits. Such states have important technological potential for quantum storage, as the coupling constants of photons to atoms can effectively be increased by a factor \sqrt{N} when coupling the atoms symmetrically to the light field [4]. Another physical realization of Dicke states is provided by angular momentum eigenstates, i.e., spin- j states arising as collective angular momentum states of $N = 2j$ physical spins-1/2. The Dicke states are formally equivalent to eigenstates $|j, m\rangle$ of operators \mathbf{J}^2 and J_z , where J_x, J_y, J_z are the usual angular momentum operators. A mixed symmetric state is then defined as a mixture of pure symmetric states (note that this notion is distinct from that of a “symmetrized mixed state,” which would be a tensor product of spin-1/2 density matrices symmetrized by summing over all permutations).

Among the pure spin- j states, spin coherent states [also called SU(2)-coherent states] are the ones that come as close as possible to the ideal of a classical phase-space point, in the sense that their quantum fluctuations for the angular momentum components are as small as allowed by Heisenberg’s uncertainty relation [5]. Furthermore, they keep this property under the dynamics induced by Hamiltonians linear in the angular momentum components, corresponding physically, for example, to precession in a magnetic field. For a spin- j coherent state, the expectation value of the angular momentum operator in a specific direction \mathbf{n} is $\langle \mathbf{J} \cdot \mathbf{n} \rangle = \hbar j$, a feature not true for a general pure spin- j state. In this sense a spin- j coherent state points in a well-defined direction (note that all

pure spin-1/2 states are coherent states, as they can be specified by a Bloch vector on the unit sphere). If a spin- j coherent state is interpreted as a symmetric N -fold tensor product of $N = 2j$ qubits, it can be expressed simply as the tensor product of N identical spin-1/2 coherent states. Therefore, spin- j coherent states coincide with symmetric separable pure states. Classical spin- j states are defined as statistical mixtures of spin coherent states [6–8]. When expressed in the Dicke basis, they can be seen as separable symmetric N -qubit states.

Just as entanglement of a quantum state can be measured as the distance to the set of separable states, the quantumness (or nonclassicality) of a spin- j state can be measured as its distance to the set of classical states [9]. Our purpose here is to investigate the quantumness properties of a state from its spectral properties. There has been substantial research trying to figure out what entanglement properties can be derived from the spectrum of eigenvalues of the density matrix representing a composite system [10–16] and how to directly access the spectrum experimentally without having to reconstruct the full density matrix [17–19]. Measures of entanglement based on the spectrum have the immediate advantages of being relatively easy to compute and being invariant under unitary transformations, i.e., capturing “absolute separability” [13]. Other well-known entanglement criteria are based on bounds of spin correlations [20,21], which in turn exploit the positive-partial-transpose (PPT) criterion. In [22] we introduced a tensorial representation for spin states. In this representation, a spin- j density matrix is expanded as a sum over matrices of dimensions $(2j + 1) \times (2j + 1)$, and the expansion coefficients take the form of a tensor $A_{\mu_1 \mu_2 \dots \mu_N}$ with $N = 2j$ indices. We showed in [23] that the PPT criteria applied to symmetric multiqubit states can be unified by means of a matrix T , obtained from the tensor representation of the equivalent spin- j state by splitting the set of indices in two subsets and considering each set as coding for the row or column index of the T matrix. The positive partial transpose is then equivalent to the positivity of the T matrix, and correlation criteria for observables, such as spin-squeezing inequalities, can also be derived from the positivity of T [23].

In light of these entanglement criteria based on the spectral properties of the density matrix or on the positivity of the

T matrix constructed from the tensor A , one may wonder whether the spectrum of the tensor A itself contains deeper information about the entanglement of the state. While the spectral theory of matrices is more than one century old, its extension to tensors is much more recent. The spectral theory of tensors has developed a lot in the past decade, and various tools have been proposed in the mathematical literature to tackle this problem (see [24] for a short review and also Sec. III). But the relevance of the spectral theory of tensors for the separability (or classicality) problem has just recently attracted some attention in the quantum information community. For example, in [25] it was shown that for pure states the largest tensor eigenvalue is equal to the geometric measure of entanglement, i.e., the maximal overlap of the state with a pure separable state. This entanglement measure is, in fact, essentially equivalent to finding the best rank-1 approximation of the tensor. Therefore, the largest tensor eigenvalue is directly related to the entanglement of a state. In this paper we will explore another connection, which relates the *smallest* tensor eigenvalue to the entanglement of a pure or mixed state. This originates from the fact that the entanglement of a state is related to the positive definiteness of a tensor, which in turn is linked to the sign of its smallest tensor eigenvalue. We show that if the smallest eigenvalue is negative, the state is entangled. If it is positive and sufficiently large, the state is separable with high probability. The latter criterion works best for relatively small values of j .

In the present paper we report the results of our investigations on the connection between the spectral properties of the tensor of order $2j$ associated with a spin- j state and the classicality of that state. The paper is organized as follows. First, we recall some definitions of quantumness and the tensor representation and show how the spectrum of the tensor is connected to the quantumness and classicality question. In Sec. III we introduce tensor eigenvalues and as an illustration calculate them explicitly for two examples. In Sec. IV we introduce an efficient algorithm for calculating the distance from a state to the set of classical states. Section V explores numerically the connection between the smallest tensor eigenvalue and quantumness.

II. DEFINITIONS

A. Entanglement and quantumness

We consider a system of N qubits, and we restrict the Hilbert space to the subspace of symmetric states. We will describe them with the terminology of spin- j states with $N = 2j$. Spin coherent states can be written as [26]

$$|\alpha\rangle = \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2} e^{-i\phi}\right)^{j-m} |j, m\rangle, \quad (1)$$

with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi[$ being spherical angles. Here $|j, m\rangle$ are the usual angular momentum basis vectors, i.e., the simultaneous eigenvectors of the total angular momentum squared \mathbf{J}^2 and its J_z component, with eigenvalues $j(j+1)$ and m , respectively ($\hbar = 1$). The spin coherent state $|\alpha\rangle$ can be seen as a spin j pointing in the direction $\mathbf{n} =$

$(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. A spin- j state ρ_c is classical if and only if it can be expressed as a mixture of spin coherent states with positive weights [7], i.e., if there exist spin coherent states $|\alpha_i\rangle$ such that

$$\rho_c = \sum_i w_i |\alpha_i\rangle\langle\alpha_i|, \quad 0 \leq w_i \leq 1, \quad \sum_i w_i = 1. \quad (2)$$

We denote by \mathcal{C} the ensemble of such states. Since a coherent spin state is formally exactly a pure symmetric separable state and vice versa [23], an entangled symmetric multiqubit state is therefore a state which cannot be written as a classical state as in Eq. (2). The amount of entanglement translates into a certain amount of nonclassicality, or quantumness, defined as the (Hilbert-Schmidt) distance to the convex set of classical states, i.e.,

$$Q(\rho) = \min_{\rho_c \in \mathcal{C}} \|\rho - \rho_c\|, \quad (3)$$

where $\|A\| = \sqrt{\text{tr}(A^\dagger A)}$ is the Hilbert-Schmidt norm [9]. A spin- j state has a quantumness larger than zero whenever the corresponding N -qubit state is entangled.

It is known that the separable state closest to a symmetric state in terms of the Bures distance is also symmetric [27]. However, for other distances this may not be the case. In particular, the Hilbert-Schmidt distance of an N -qubit symmetric state to the set of separable states is, in general, not equal to the quantumness of the corresponding state of a physical spin- j system, as some separable nonsymmetric states may lie closer.

B. Tensor representation

In order to conveniently deal with expansions of quantum states over spin coherent states, we use a representation suited to this purpose that has recently been introduced in [22]. We express a spin- j density matrix ρ in the following way. Let σ_a , $1 \leq a \leq 3$, be the usual Pauli matrices and σ_0 be the 2×2 identity matrix. We define the 4^N matrices $S_{\mu_1 \dots \mu_N}$ (with $N = 2j$) by

$$S_{\mu_1 \dots \mu_N} = P(\sigma_{\mu_1} \otimes \sigma_{\mu_2} \cdots \otimes \sigma_{\mu_N}) P^\dagger, \quad 0 \leq \mu_i \leq 3, \quad (4)$$

with P being the projector onto the symmetric subspace of tensor products of N spins- $\frac{1}{2}$ (the subspace spanned by Dicke states). The matrix ρ can be expanded over $S_{\mu_1 \dots \mu_N}$ as

$$\rho = \frac{1}{2^N} A_{\mu_1 \mu_2 \dots \mu_N} S_{\mu_1 \mu_2 \dots \mu_N} \quad (5)$$

(summation over repeated indices is implicit), with real coefficients

$$A_{\mu_1 \mu_2 \dots \mu_N} = \text{tr}(\rho S_{\mu_1 \mu_2 \dots \mu_N}) \quad (6)$$

(see [22] for details). $A_{\mu_1 \mu_2 \dots \mu_N}$ are invariant under permutation of the indices and enjoy the property that for any μ_i , $3 \leq i \leq N$ and $0 \leq \mu_i \leq 3$,

$$\sum_{a=1}^3 A_{a a \mu_3 \dots \mu_N} = A_{0 0 \mu_3 \dots \mu_N}. \quad (7)$$

Normalization of the states ρ in (5), $\text{tr} \rho = 1$, translates to $A_{0 \dots 0} = 1$.

The coordinates $A_{\mu_1\mu_2\cdots\mu_N}$ can be seen as a symmetric order- N tensor. We thus refer to (6) as the tensor representation of ρ . This representation is a generalization of the spin- $\frac{1}{2}$ Bloch sphere representation

$$\rho = \frac{1}{2} A_\mu S_\mu, \quad (8)$$

with Bloch vector $\mathbf{A} = \text{tr}(\rho \boldsymbol{\sigma})$ and $A_0 = 1$ (noting that $S_\mu = \sigma_\mu$).

C. Classicity in the tensor representation

The tensor associated with a spin coherent state $|\alpha\rangle$ pointing in direction \mathbf{n} is simply given by

$$A_{\mu_1\mu_2\cdots\mu_N} = \langle \alpha | S_{\mu_1\mu_2\cdots\mu_N} | \alpha \rangle = n_{\mu_1} n_{\mu_2} \cdots n_{\mu_N}, \quad (9)$$

with $n_0 = 1$ and $\mathbf{n} = (n_1, n_2, n_3)$ [22]. The definition of classicality, Eq. (2), can be reexpressed in terms of tensors. A state is classical if and only if there exist positive weights w_i and unit vectors $\mathbf{n}^{(i)}$ such that its tensor of coordinates A can be written as

$$A_{\mu_1\mu_2\cdots\mu_N} = \sum_i w_i n_{\mu_1}^{(i)} n_{\mu_2}^{(i)} \cdots n_{\mu_N}^{(i)}, \quad (10)$$

with $n_\mu^{(i)} = (1, \mathbf{n}^{(i)})$. Contracting such a tensor with an arbitrary real order-1 tensor q gives

$$A_{\mu_1\mu_2\cdots\mu_N} q_{\mu_1} q_{\mu_2} \cdots q_{\mu_N} = \sum_i w_i (n_\mu^{(i)} q_\mu)^N. \quad (11)$$

If j is an integer (i.e., if N is even), the right-hand side is always positive since the weights w_i are positive. Therefore, any tensor having the form (10) is such that its contraction with an arbitrary order-1 tensor is positive. This precisely corresponds to the definition of positive semidefiniteness of the tensor A as introduced in [28]. A necessary condition for classicality of ρ is thus that its associated tensor be positive semidefinite. In the case of a spin-1 system, where the tensor reduces to a matrix, this is also a sufficient condition [29]. However, for $j \geq 2$ it is not sufficient anymore since there exist nonclassical states which have a positive tensor representation, as will be discussed below.

Before continuing the discussion of the relationship between classicality and tensor properties, we introduce some elements of the spectral theory of tensors.

III. TENSOR EIGENVALUES

A. Definitions

Let $A_{\mu_1\cdots\mu_N}$ be the tensor representation of a spin- j state. Its entries are real and symmetric under any permutation of indices. Tensor eigenvalues and eigenvectors of such a real symmetric tensor are defined in [28]. Different definitions have been introduced. For instance, for a tensor with N indices, each ranging from 0 to $n-1$ (in our case $n=4$), Z eigenvalues, which we will use in this paper, are the real numbers λ such that there exists a real vector v with n components verifying

$$\begin{aligned} Av^{[N-1]} &= \lambda v, \\ v^T v &= 1, \end{aligned} \quad (12)$$

where $Av^{[k]}$ denotes the tensor of order $N-k$ given by

$$(Av^{[k]})_{\mu_{k+1}\cdots\mu_N} = A_{\mu_1\mu_2\cdots\mu_N} v_{\mu_1} v_{\mu_2} \cdots v_{\mu_k} \quad (13)$$

and v^T is the transpose of v .

The different definitions of tensor eigenvalues can be written as special cases of the B eigenvalues, which are defined [30] as

$$Av^{[N-1]} = \lambda Bv^{[m-1]}, \quad Bv^{[m]} = 1, \quad (14)$$

where B is a real symmetric order- m tensor and $\lambda, v_\mu \in \mathbb{C}$. If B is chosen as the identity matrix (i.e., $m=2$) and λ, v_μ are restricted to real values, then the solutions λ are the Z eigenvalues defined in Eq. (12). If $m=N$ and B is the identity tensor (i.e., $B_{\mu_1\cdots\mu_n} = 1$ if all μ_i are identical and $B_{\mu_1\cdots\mu_n} = 0$ otherwise), so that $Bx^{[m]} = x_0^m + x_1^m + \cdots + x_n^m$, real solutions to (14) are called H eigenvalues [28]. Another type is the D eigenvalues, which have recently found application in magnetic resonance imaging studies of the diffusion kurtosis coefficients of water molecules [31]. They can be written as real B eigenvalues if $m=2$ and there exists a symmetric positive-definite matrix $D \in \mathbb{R}^{n \times n}$ with $Bx^{[2]} = x^T D x$, such that there exists a real vector v with

$$Av^{[m-1]} = \lambda Dv, \quad v^T Dv = 1. \quad (15)$$

For a more detailed overview on the topic of tensor eigenvalues see [24,28,32].

It is possible, via resultant theory, to generalize the usual matrix notions of the determinant and of the characteristic polynomial and to obtain eigenvalues as the (generally complex) roots of the characteristic polynomial associated with the tensor [28]. Note, however, that the Z (or H) eigenvalues defined above are real numbers. If this restriction to real numbers is lifted, many properties of ordinary matrix eigenvalues are recovered (for instance, the number of eigenvalues, or their total sum, is known). Nevertheless, the restriction to real numbers is justified if one wants to generalize the property that a matrix is positive semidefinite if and only if its eigenvalues are positive. Indeed, both Z and H eigenvalues share the property that a tensor is positive semidefinite if and only if all Z or H eigenvalues are positive, which makes them the most natural suitable generalization of matrix eigenvalues. But the H eigenvalues are not invariant under rotation, while Z eigenvalues are, as will be shown below. Since spin coherent states behave in a very simple way under rotation, we will concentrate on the Z eigenvalues defined by Eq. (12), which we will refer to, from now on, as ‘‘tensor eigenvalues.’’ Note that we also tested our methods on the H eigenvalues, and they gave results comparable to the ones presented in Sec. V.

B. Properties

Tensor eigenvalues do not share all the properties of the familiar matrix eigenvalues. For example, it is, in general, not true that the tensor eigenvalues of a diagonal tensor are just its diagonal elements. However, the tensor eigenvalues are invariant under rotations, and the corresponding eigenvectors are just the rotated eigenvectors (Theorem 7 of [28]). In order to familiarize the reader with the tensor notation, let us show this explicitly. Take v as a tensor eigenvector of the real symmetric tensor A with tensor eigenvalue λ , i.e., fulfilling (12). Given a

real orthogonal matrix R and the rotated objects marked with primes, then

$$A'v'^{[N-1]} = \prod_{i=1}^N R_{\mu_i, v_i} A_{v_1 \dots v_N} \prod_{j=1}^{N-1} R_{\mu_j, \eta_j} v_{\eta_j} \quad (16)$$

$$= \prod_{j=1}^{N-1} (R^T R)_{v_j, \eta_j} R_{\mu_N, v_N} A_{v_1 \dots v_N} v_{\eta_j} \quad (17)$$

$$= R_{\mu_N, v_N} A_{v_1 \dots v_N} \prod_{j=1}^{N-1} v_{\eta_j} \stackrel{(12)}{=} R_{\mu_N, v_N} \lambda v_{v_N} = \lambda v', \quad (18)$$

which proves that the eigenvalues are unchanged by rotations and the new eigenvectors are just the rotated old ones. This feature is particularly important in our case because a rotated spin- j quantum state $\rho' = \hat{R}^\dagger \rho \hat{R}$, with $\hat{R} = \exp(-i\theta \mathbf{J} \cdot \mathbf{n})$ being the spin- j representation of a rotation, has a tensor representation given by $A'_{\mu_1 \dots \mu_N} = R_{\mu_1, v_1} \dots R_{\mu_N, v_N} A_{v_1 \dots v_N}$, with R being the 4×4 matrix whose 3×3 lower right block is the orthogonal matrix associated with the rotation of axis \mathbf{n} and angle θ and $R_{\mu, 0} = R_{0, \mu} = \delta_{0, \mu}$ [22].

Determining tensor eigenvalues is usually a computationally hard problem. It can be expressed in the following way: The tensor eigenvalues defined by (12) are the critical points of the polynomial

$$L(\lambda; x_1, x_2, \dots, x_N) = Ax^{[N]} - \lambda(|\mathbf{x}|_2^N - 1), \quad (19)$$

with

$$|\mathbf{x}|_2 = \sqrt{x_0^2 + x_1^2 + x_2^2 + x_3^2}. \quad (20)$$

Indeed, critical points of L are defined by $\nabla L = 0$; the conditions $\partial L / \partial x_v = 0$ are equivalent to the first line in Eq. (12), as can easily be seen from the fact that if A is a symmetric tensor, one has

$$\frac{\partial}{\partial x_v} Ax^{[N]} = N(Ax^{[N-1]})_v \quad (21)$$

and

$$\frac{\partial}{\partial x_v} |\mathbf{x}|_2^N = N(x_0^2 + x_1^2 + x_2^2 + x_3^2)^{N/2-1} x_v. \quad (22)$$

Condition $\partial L / \partial \lambda = 0$ gives the second line in Eq. (12). Thus, the tensor eigenvalues can be obtained as the local extrema of $Ax^{[N]}$ over the three-sphere $x_0^2 + x_1^2 + x_2^2 + x_3^2 = 1$.

As shown in [33], a real symmetric tensor is positive semidefinite, i.e., $Ax^{[N]} \geq 0$ for all x , if and only if all of its tensor eigenvalues are non-negative. Hence, it is sufficient to calculate the smallest tensor eigenvalue to determine the positivity of the tensor. In particular, a tensor can be positive definite only if the tensor has an even number of indices: Otherwise, each tensor eigenpair (λ, v) also has a negative counterpart $(-\lambda, -v)$, as can be seen by the definition (12). Numerically, the smallest tensor eigenvalue is obtained by computing the global minimum of $Ax^{[N]}$ over the three-sphere. Such a problem can be tackled numerically using methods described, e.g., in [30]. In the next section we show examples of quantum states where tensor eigenvalues can be derived analytically.

C. Examples

1. Tensor eigenvalues of spin coherent states

For a spin- j coherent state with Bloch vector \mathbf{n} the tensor representation $A_{\mu_1 \dots \mu_N}$ takes the simple form (9). In order to deduce all tensor eigenvalues λ and eigenvectors x_μ , we have to solve Eq. (12), which then reads

$$A_{\mu_1 \dots \mu_N} x^{[N-1]} = (n_{\mu_1} x_{\mu_1}) \dots (n_{\mu_{N-1}} x_{\mu_{N-1}}) n_{\mu_N} \\ = \lambda x_{\mu_N}, \quad |\mathbf{x}|_2 = 1. \quad (23)$$

Since the tensor eigenvalues are invariant under rotation, we can, without loss of generality, rotate \mathbf{n} to the form $(1, 0, 0)$. This simplifies Eq. (23) to

$$(x_0 + x_1)^{N-1} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \lambda \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad |\mathbf{x}|_2 = 1. \quad (24)$$

From the third and fourth lines it is clear that there are two solutions, $\lambda = 0$ or $x_2 = x_3 = 0$. If $\lambda = 0$, then $x_0 = -x_1$, and x_2, x_3 are arbitrary under the restriction $|\mathbf{x}|_2 = 1$. Otherwise, $\lambda = \sqrt{2}^N$ for even N or $\lambda = \pm \sqrt{2}^N$ for odd N , and $x_0 = x_1 = \pm 1/\sqrt{2}, x_2 = x_3 = 0$. Thus, the tensor eigenvalues of a tensor associated with a coherent spin- j state are $(\pm 1)^N 2^j$ and 0. For integer j we recover the fact that the tensor is positive, as it should be since a spin coherent state is classical.

2. Tensor eigenvalues of the maximally mixed state

For the maximally mixed state $\rho_0 = \frac{1}{N+1} \mathbb{1}_{N+1}$, the tensor representation is given by

$$Ax^N = \sum_{k=0}^{\lfloor j \rfloor} \frac{\binom{N}{2k}}{2k+1} x_0^{2(j-k)} (x_1^2 + x_2^2 + x_3^2)^k, \quad (25)$$

where $\lfloor \cdot \rfloor$ is the floor function [22]. For vectors \mathbf{x} constrained by $x_0^2 + x_1^2 + x_2^2 + x_3^2 = 1$, Eq. (25) can be rewritten as

$$Ax^N = \sum_{k=0}^{\lfloor j \rfloor} \frac{\binom{N}{2k}}{2k+1} x_0^{2(j-k)} (1 - x_0^2)^k := g(x_0), \quad (26)$$

with $-1 \leq x_0 \leq 1$. If j is an integer, $g(x_0)$ is a sum of positive terms and thus larger than zero. The tensor eigenvalues are local extrema of Ax^N on the three-sphere, or, equivalently, the local extrema of $g(x_0)$ over the interval $[-1, 1]$. The local extrema on the border of the interval, $|x_0| = 1$, give a tensor eigenvalue $\lambda = 1$. Because $g(x_0)$ is symmetric, there is a local extremum at $x_0 = 0$, which gives the tensor eigenvalue $\lambda = 1/(N+1)$. For $j \geq 3$ the function $g(x_0)$ has exactly one extremum in the interval $]0, 1[$, which gives a third tensor eigenvalue (see the Appendix for a proof). Thus, for integer j the tensor associated with the maximally mixed state has three tensor eigenvalues, and the minimal tensor eigenvalue is $\lambda_{\min} = 1/(N+1)$.

For half integer j there are two tensor eigenvalues on the border of the interval which give ± 1 . For $j \geq 5/2$ the function $g(x_0)$ has a maximum in $]0, 1[$ (see the Appendix for a proof) and, since $g(x_0)$ is antisymmetric, also a corresponding minimum in $] -1, 0[$. Thus, the tensor has four tensor eigenvalues.

IV. CALCULATING QUANTUMNESS

Our goal is to compare quantumness of a spin- j state as measured by the distance (3) with spectral properties of the tensor associated with it. In order to compute quantumness (3) efficiently, the calculation can be rewritten as a quadratic optimization problem by fixing a large number of spin coherent states in the sum (2) and optimizing over the weights w_i . This is detailed in Sec. IV A. However, this does not guarantee finding the global minimum, as the decompositions of the closest classical states may involve spin coherent states which do not belong to the large set chosen. To improve the accuracy of the estimation we will use the outcome of the quadratic optimization as a starting point in a linear optimization routine detailed in Sec. IV B.

A. Quadratic algorithm

The state is written as a $[2(N+1)^2]$ -dimensional real vector \mathbf{r} , whose entries are the real and imaginary entries of its density matrix ρ in the $|j, m\rangle$ basis (or any other fixed basis). In the same way the classical state ρ_c in Eq. (2) is written as $C\mathbf{w}$, where C is a $[2(N+1)^2] \times M$ real matrix whose i th column is given by the real and imaginary parts of entries of $|\theta_i, \phi_i\rangle\langle\theta_i, \phi_i|$ expressed in the same basis as ρ , \mathbf{w} is the vector of weights, and M is the number of spin coherent states used in the sum of the form of Eq. (2). The squared quantumness can be written as

$$Q^2(\rho) = \min_{C, \mathbf{w}} \sum_{i=1}^{2(N+1)^2} [r_i - (C\mathbf{w})_i]^2, \quad (27)$$

which can be expressed as

$$Q^2(\rho) = \min_{C, \mathbf{w}} [\mathbf{w}^T (C^T C) \mathbf{w} - (2\mathbf{r}^T C) \mathbf{w} + \mathbf{r}^T \mathbf{r}]. \quad (28)$$

To approximate the solution to this optimization problem we generate a large set of M (~ 800) spin coherent states $|\theta_i, \phi_i\rangle$ that determine a matrix C and a vector $\mathbf{c} = (\mathbf{r}^T C)$ and solve

$$\min_{\mathbf{w}} \mathbf{w}^T (C^T C) \mathbf{w} - 2\mathbf{c}^T \mathbf{w}, \quad w_i \geq 0 \quad (29)$$

(we removed the constant term $\mathbf{r}^T \mathbf{r}$). Note that the entries of $(C^T C)$ are given by

$$\begin{aligned} (C^T C)_{ik} &= |\langle\theta_i, \phi_i|\theta_k, \phi_k\rangle|^2 \\ &= 4^{-j} [1 + \cos \theta_i \cos \theta_k \\ &\quad + \cos(\phi_i - \phi_k) \sin \theta_i \sin \theta_k]^{2j} \end{aligned} \quad (30)$$

and that

$$\mathbf{c}_i = \langle\theta_i, \phi_i|\rho|\theta_i, \phi_i\rangle. \quad (31)$$

The optimization (29) can be performed with the powerful numerical algorithms available, e.g., the ‘‘interior-point-convex’’ method [34]. It is notable that the size of the quadratic optimization problem, given by the vector \mathbf{c} and the matrix $C^T C$, does not depend on the spin size j but only on the number of random spin coherent states used. However, for very large values of j (~ 1000) even the one-time calculation of \mathbf{c} and $C^T C$ can become computationally expensive.

To improve the outcome it is advantageous to iterate the optimization several times with different sets of spin coherent states. In the subsequent iterations, only the spin coherent

states with large weights are kept, and additional nearby states are added to the set. The set is then completed with random spin coherent states. After typically around eight iterations, we take the best outcome as an approximation of the global minimum of (27). This also provides an approximation $\tilde{\rho}_c$ of the true closest classical state ρ_c . By construction, $\tilde{\rho}_c$ is a classical state, so that quantumness is necessarily overestimated since the distance to any classical state gives an upper bound on the quantumness. To further improve its determination, a linear optimization can then be performed as follows.

B. Linear algorithm

Suppose we have obtained an approximation $\tilde{\rho}_c$ for the closest classical state ρ_c by running the quadratic algorithm above. If the classical state $\tilde{\rho}_c$ is not exactly on the border of the classical domain, it is possible to move it in the direction of the state ρ while remaining in the classical domain. This yields a better approximation of the global minimum and thus of the actual quantumness. This step can be formulated as a linear optimization problem by parametrizing the states in between the classical state $\tilde{\rho}_c$ and ρ as

$$\rho_k = (1-k)\tilde{\rho}_c + k\rho = \tilde{\rho}_c + k(\rho - \tilde{\rho}_c), \quad (32)$$

with $k \in [0, 1]$. Now the optimization task is to maximize k under the constraint that ρ_k stays classical, which can be formulated in the form of linear constraints as

$$\sum_i w_i |\theta_i, \phi_i\rangle\langle\theta_i, \phi_i| + k(\tilde{\rho}_c - \rho) = \tilde{\rho}_c, \quad (33)$$

and the optimization is now performed on w_i and k , with $0 \leq w_i \leq 1$ and $k > 0$, while $|\theta_i, \phi_i\rangle$ are (a large number of) fixed spin coherent states. Like in Sec. IV A, this optimization problem can be written as

$$\max_{\mathbf{w}, k} k, \quad C\mathbf{w} + (\tilde{\mathbf{r}}_c - \mathbf{r})k = \tilde{\mathbf{r}}_c, \quad (34)$$

where the i th columns of C are given by the real and imaginary parts of entries of $|\theta_i, \phi_i\rangle\langle\theta_i, \phi_i|$ and $\mathbf{r}, \tilde{\mathbf{r}}_c$ are the real and imaginary parts of entries of the density matrices ρ and $\tilde{\rho}_c$. Since a linear optimization is much faster than a quadratic optimization, the set of random spin coherent states used to fix the linear constraints can be much larger, e.g., usually by two orders of magnitude, and still have a run time comparable to the quadratic optimization. However, in contrast to the quadratic algorithm the computational demands depend on the spin size j since the number of rows in C scales as $O(j^2)$. In the results presented in the next section this linear optimization step improves the quadratic results for $Q(\rho)$ usually by an absolute amount smaller than 10^{-4} . While this improvement is usually negligible, it becomes relevant for estimating quantumness of states close to the boundary of classical states and to properly identify classical states.

V. CONNECTION BETWEEN TENSOR EIGENVALUES AND QUANTUMNESS

A. Tensor eigenvalues for entanglement detection

As mentioned earlier, a classical state must have a positive-semidefinite tensor representation. Therefore, if its smallest tensor eigenvalue λ_{\min} is negative, the state is detected as

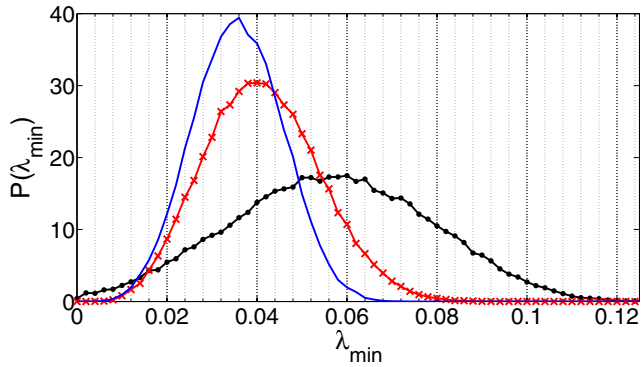


FIG. 1. Probability distribution of the smallest tensor eigenvalue λ_{\min} for random states on the border of the classical domain, with $j = 2$ (black dots), $j = 3$ (red crosses), and $j = 4$ (blue solid line). These states are the closest classical states to random mixed states and were determined with the quadratic and linear algorithms described in Sec. IV.

nonclassical, i.e., entangled. To test the rigor of the detection we generated states just on the border of the set of classical states. This was done by taking random states drawn from the Hilbert-Schmidt ensemble of matrices $\rho = GG^\dagger/\text{tr}(GG^\dagger)$, with G being a complex matrix with independent Gaussian entries (see [35] for details), and calculating its closest classical state according to the method presented in the previous section. In Fig. 1 the distribution of the smallest eigenvalues is shown for this ensemble of closest classical states. If positivity of A were a sufficient condition for classicality, then λ_{\min} would be equal to zero for all closest classical states. Numerically, we rather get values centered around 0.03, 0.04, and 0.06 for $j = 4, 3, 2$, respectively.

Thus, states lying at the border of classical states, with zero quantumness, have a smallest tensor eigenvalue significantly larger than zero, which indicates that for the values of j

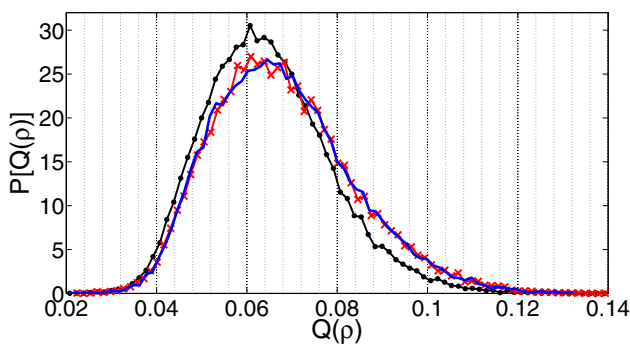


FIG. 2. Probability distribution of the quantumness $Q(\rho)$ (3) for states having a positive smallest tensor eigenvalue smaller than 10^{-5} . The states are created by mixing a random mixed state with the maximally mixed state according to (35) and decreasing a until the smallest tensor eigenvalue is close to zero. The numerical uncertainty of the quantumness is of the order of 10^{-4} . The black line with circles, red line with crosses, and blue solid line correspond to spin sizes $j = 2, 3, 4$. These states are all entangled but nevertheless have a positive definite tensor representation.

considered this method of entanglement detection is not well suited for too weakly entangled states.

Conversely, one may wonder what is the typical quantumness of states which have a vanishing smallest tensor eigenvalue. To investigate this we generated states such that $\lambda_{\min} \simeq 0$ by mixing a random initial state ρ with the maximally mixed state

$$a\rho + (1 - a)\frac{1}{N + 1}\mathbb{1}, \quad 0 \leq a \leq 1 \quad (35)$$

(with $\mathbb{1}$ being the identity matrix), and decreasing a until the smallest tensor eigenvalue was close to zero. The results for these states are shown in Fig. 2. The quantumness is distributed

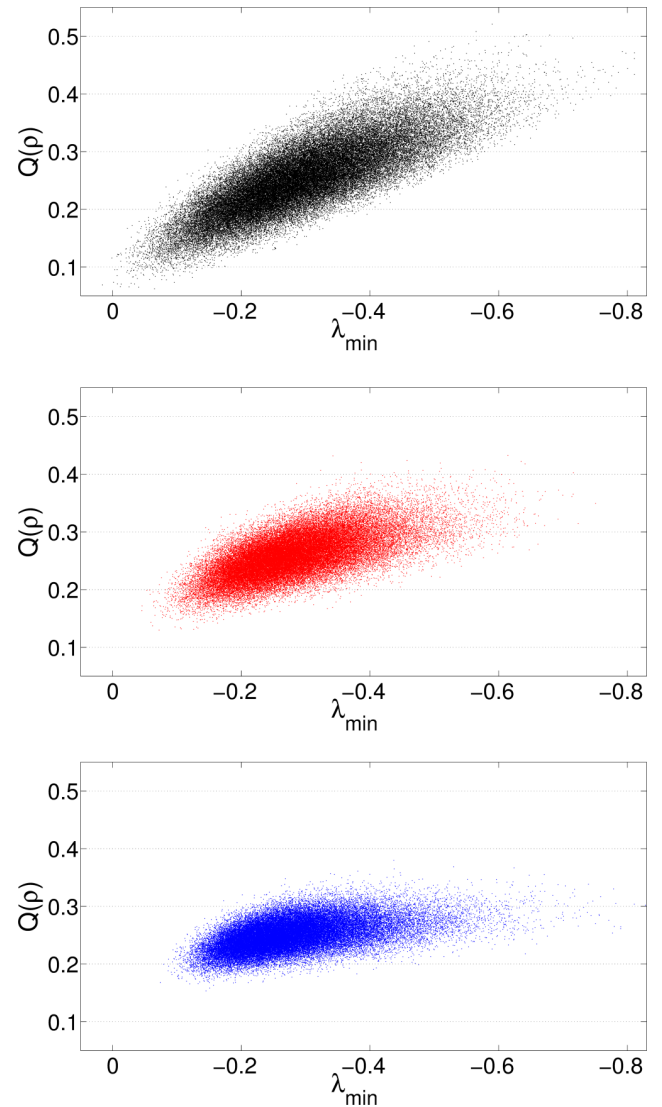


FIG. 3. The quantumness (3) as a function of the smallest tensor eigenvalue (12) for $\sim 60\,000$ randomly generated mixed spin- j states. The top panel corresponds to spin size $j = 2$, the middle panel corresponds to $j = 3$, and the bottom panel corresponds to spin size $j = 4$. There is a clear correlation between the amount of quantumness and the magnitude of the negative smallest tensor eigenvalue; however, this correlation gets weaker for $j = 3$ and even weaker for $j = 4$.

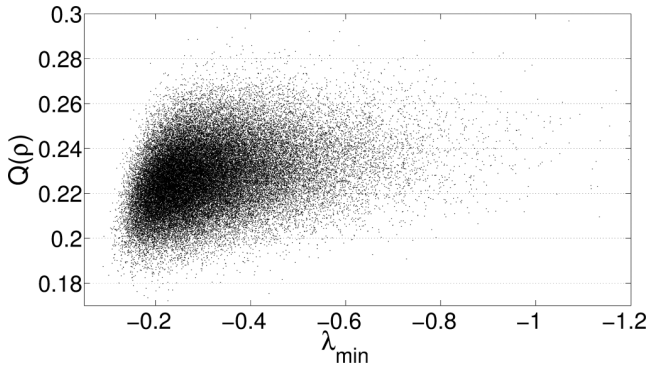


FIG. 4. The quantumness (3) of $\sim 60\,000$ randomly generated spin-6 mixed states as a function of their smallest tensor eigenvalue (12). For this system size there is almost no correlation between the magnitude of the smallest tensor eigenvalue and the quantumness.

around the value of 0.06, irrespective of the spin size j , which again indicates that the smallest tensor eigenvalue is not able to detect weakly entangled states. This appears to be a systematic underperformance because we did not find instances of classical states which also have a smallest tensor eigenvalue equal to zero. Instead, almost all states on the “detection border” $\lambda_{\min} = 0$ already have a quantumness larger than 0.02.

To conclude, the smallest tensor eigenvalue detects entanglement (or quantumness) in spin-2 to spin-4 states reliably only if the quantumness is at least about 0.1. In the other direction, spin-2 to spin-4 states can be assumed to be separable (or classical) only if the smallest tensor eigenvalue is larger than 0.12.

B. Measure of entanglement based on tensor eigenvalues

The results above show that while any state with $\lambda_{\min} < 0$ is entangled, the positivity of λ_{\min} does not seem to be a good indicator of separability. However, for nonclassical states, the amount by which λ_{\min} is negative is correlated with the amount of entanglement as measured by the quantumness.

This is an approach similar to that for the entanglement measure of negativity [36], where the amount of entanglement is taken as the sum of all negative eigenvalues of the partially transposed state ρ^{PT} , namely,

$$\mathcal{N}(\rho) = \sum_i \frac{|\mu_i| - \mu_i}{2}, \quad (36)$$

where μ_i are the eigenvalues of ρ^{PT} . For $j = 1$, we showed in [23] that the tensor eigenvalues are exactly the eigenvalues of ρ^{PT} . Unfortunately, in the case of tensor eigenvalues ($j \geq 3/2$), it is computationally expensive to find all tensor eigenvalues. But the smallest tensor eigenvalue provides at least an indicator of the amount of entanglement. This is illustrated in Fig. 3, where quantumness is plotted as a function of the smallest tensor eigenvalue (computed by the algorithms described in Sec. IV) for a large set of random states. The correlation between the two quantities gets weaker for larger system sizes, i.e., $j \geq 4$. For spin $j = 6$, the correlation is almost gone, as can be seen in Fig. 4.

VI. CONCLUSION

We introduced a connection between the mathematical concept of tensor eigenvalues and the study of entanglement. The smallest tensor eigenvalue can be used to detect quantumness in symmetric states and can also give an estimator of its amount. Interestingly, this extends previous results in the mathematical literature relating the largest tensor eigenvalue to the geometric measure of entanglement. If the smallest tensor eigenvalue is negative, the state is detected as entangled. In the case of spin-1 the positivity of the smallest tensor eigenvalue is even a necessary and sufficient separability criteria. For $j \geq 2$ the correlation between the amount of quantumness and the magnitude of the (negative) smallest tensor eigenvalue is noticeable for $j = 2, 3, 4$, but for higher values of j quantumness and magnitude of the smallest tensor eigenvalue are almost uncorrelated.

In regard to detecting separability, a state can be assumed to be classical if the smallest tensor eigenvalue is larger than 0.12. However, for $j \geq 2$ and $0 \leq \lambda_{\min} < 0.12$, entangled states are not detected with high probability, rendering the criteria less useful in this regime. This is due to the fact that weakly entangled states usually have a positive-semidefinite tensor representation (and are therefore not detected by the smallest tensor eigenvalue criterion).

A possible way to improve these results might be to use the sum of all negative tensor eigenvalues as an estimator for the quantumness of a state, instead of just the smallest tensor eigenvalue. However, the calculation of all tensor eigenvalues is computationally much more demanding.

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APPENDIX: TENSOR EIGENVALUES OF THE MAXIMALLY MIXED STATE

Here we will prove that the function $g(x)$ defined in (26) has only one local extremum in the open interval $]0, 1[$ for $j \geq \frac{5}{2}$. We reparametrize the function g with

$$x \rightarrow \frac{\cos t + \sin t}{\sqrt{2}}, \quad (A1)$$

with $t \in]\frac{\pi}{4}, \frac{3\pi}{4}[$, so that we get

$$g(x) \rightarrow f(t) = \frac{2^j \cos^{2j+1} t - \sin^{2j+1} t}{2j+1 \cos t - \sin t}. \quad (A2)$$

The condition $f'(t) = 0$ is equivalent to $H(t) = 0$, with

$$H(t) := (\sin t + \cos t)(\cos^k t - \sin^k t) + k \sin t \cos t \times (\sin t - \cos t)(\cos^{k-2} t + \sin^{k-2} t), \quad (A3)$$

with $k = 2j + 1$. Using $H(\pi/4) = 0$ and $H(3\pi/4) \leq 0$, we show that $H(t)$ has only one real root in the interval $]\frac{\pi}{4}, \frac{3\pi}{4}[$ by showing that it is strictly increasing, then strictly decreasing, then strictly increasing over this interval for $j \geq \frac{5}{2}$.

To find the extreme points of $H(t)$ we calculate

$$H'(t) = (k-1)(\cos t - \sin t) \times \left[\sin^k t - \cos^k t + k \left(\tan^2 t \cos^k t - \frac{\sin^k t}{\tan^2 t} \right) \right]. \quad (\text{A4})$$

Now we show that $H'(t)$ has two roots in $]\frac{\pi}{4}, \frac{3\pi}{4}[$ by setting $u = \cot t$ in (A4) with $u \in]-1, 1[$ and counting the roots of

$$P(u) := -u^k + ku^{k-2} - ku^2 + 1 \quad (\text{A5})$$

in the interval $]-1, 1[$. Descartes's rule of signs tells us that this function has either three or one roots in $]0, \infty[$. As $P(0) = 1$, $P(1) = 0$, $P'(1) = k(k-5) > 0$, and $\lim_{u \rightarrow \infty} P(u) = -\infty$, there are necessarily three roots in $]0, \infty[$ and exactly one in $]0, 1[$. To study the negative side $u < 0$, note that if k is even,

the function $P(u)$ is symmetric, so that there is also only one root in $u \in]-1, 0[$. In the case of odd k , we set $w = -u \in]0, 1[$, and

$$P(-u) = \tilde{P}(w) = w^k - kw^{k-2} - kw^2 + 1. \quad (\text{A6})$$

Applying Descartes's rule again to \tilde{P} , we get that $\tilde{P}(w)$ has either two or zero real roots in $]0, \infty[$. However, since $\tilde{P}(0) = 1$, $\tilde{P}(1) = 2(1-k) < 0$ and $\lim_{w \rightarrow \infty} \tilde{P}(w) = \infty$, the function has to have exactly one root in the interval $]0, 1[$ and one in $]1, \infty[$.

This shows that $H'(t)$ has one root in $]\pi/4, \pi/2[$ and one in $]\pi/2, 3\pi/4[$. Since $H'(\pi/2) = 1 - k < 0$, we conclude that $H(t)$ increases, decreases, and then increases again, so that it has only one root in $]\pi/4, 3\pi/4[$. So $g(x)$ defined in (26) also has only one extreme point in the open interval $]0, 1[$, which gives a single tensor eigenvalue $x \in]0, 1[$.

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A.4. Absolutely classical spin states

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Absolutely classical spin statesF. Bohnet-Waldraff,^{1,2} O. Giraud,¹ and D. Braun²¹*LPTMS, CNRS, Université Paris-Sud, Université Paris-Saclay, 91405 Orsay, France*²*Institut für Theoretische Physik, Universität Tübingen, 72076 Tübingen, Germany*

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We introduce the concept of “absolutely classical” spin states, in analogy to absolutely separable states of bipartite quantum systems. Absolutely classical states are states that remain classical (i.e., a convex sum of projectors on coherent states of a spin j) under any unitary transformation applied to them. We investigate the maximal size of the ball of absolutely classical states centered on the maximally mixed state and derive a lower bound for its radius as a function of the total spin quantum number. We also obtain a numerical estimate of this maximal radius and compare it to the case of absolutely separable states.

DOI: [10.1103/PhysRevA.95.012318](https://doi.org/10.1103/PhysRevA.95.012318)**I. INTRODUCTION**

The rise of quantum information technology has led to the need to classify and quantify the resources that ultimately enable a quantum advantage in certain computational, communicational, or metrological tasks. Most of the efforts have concentrated on classifying entanglement. Indeed, entanglement has been recognized to be necessary for, e.g., computational speedups (at least for pure states) [1], quantum teleportation [2], superdense coding [3], and quantum data hiding [4]. It can also be used for quantum key distribution [5] or for achieving enhanced precision in certain metrological applications [6]. Recently, it has been realized that other types of quantum mechanical correlations in the form of “quantum discord” exist that do not require entanglement but may still have useful applications [7].

Quantum entanglement necessarily requires at least bipartite systems. However, even for a single system, one can meaningfully ask to what extent a particular quantum state shows genuine quantum mechanical properties. In quantum optics, such questions were investigated at least as early as the middle of the last century. Quasiprobability distributions were introduced that allow one to distinguish “classical” quantum states from states that show genuine quantum effects such as enhanced quantum fluctuations of observables, or quantum interference, including multiphoton interference. An important role is played by coherent states of the radiation field, in which the quantum fluctuations of the field quadratures are minimal and evenly distributed over the canonical coordinates. Such states come as close as quantum mechanically possible to a point in classical phase space and, in general, one can consider states that can be expressed as a convex sum (i.e., a classical mixture) of (projectors onto) coherent states as classical [8,9]. Recently, these ideas were transferred to spin states, where SU(2) coherent states (introduced in [10]) play the role of the most classical pure states, and a mixed spin state is considered “classical” if it can be written as a statistical mixture of SU(2) coherent states [11]. With this classification, all states of a spin 1/2 are classical as they can be expressed as classical mixtures of pure states with minimal quantum fluctuations. For a spin 1, there are genuinely nonclassical states, and necessary and sufficient conditions are known for classicality. These conditions can be used to explore analytically the geometry of quantum states [12] and provide a full analytical

parametrization of the classical domain [13]. For higher values of j , one can find sufficient conditions for nonclassicality from the positivity of correlation functions of spin observables [11,14]. By definition, the classical states form a convex set, and one can define a “quantumness” measure of a state as the distance from this state to the convex set of classical states, in analogy to geometric measures of entanglement [15,16]. Indeed, the two problems are related through the fact that spin- j states can also be understood as states of $N = 2j$ spins 1/2 that are fully symmetric under permutation of particles, so that quantumness of a spin j is equivalent to entanglement of $N = 2j$ spins 1/2 in the fully symmetric sector of the Hilbert space of N two-level systems [14].

Any measure of entanglement $E(\rho)$ is by definition invariant under local unitary operations. But one can also ask for states for which $E(\rho)$ is invariant under *any* unitary operation. In particular, states ρ such that $E(U\rho U^\dagger) = 0$ for all unitary operations U , called “absolutely separable” states, have attracted substantial interest [17–23]. Absolutely separable states have the property that no entanglement can be created from them, no matter how strongly and how long the corresponding particles interact. Conversely, for states which are not absolutely separable, there is at least in principle the possibility that some entanglement be created from a common unitary evolution. The maximally mixed state ρ_0 , which is proportional to the identity matrix, is obviously an absolutely separable state. As separable states form a closed set, there is a ball around ρ_0 such that all states within that ball are absolutely separable. Finding the largest radius of such a ball provides a sufficient condition for absolute separability; such a question was addressed in [20].

In the present work, we ask an analogous question for quantumness: what are the states of a spin j that remain classical no matter what unitary evolution is applied to them? These states have the physical interpretation that no quantumness can be created from them in the course of any unitary time evolution, generated by an arbitrary, even time-dependent Hamiltonian. We correspondingly call these states “absolutely classical.” Alternatively, states that are not absolutely classical have the potential that in the course of some unitary evolution, some quantumness may appear.

The aim of the paper is to provide a characterization of the set of absolutely classical states in terms of a maximum

distance from the maximally mixed spin- j state, such that any state closer to the fully mixed state is guaranteed to be classical. This distance is the maximal radius that a ball of classical states around the maximally mixed spin- j state can have. We provide a lower bound for this maximum radius based on an expansion of the Glauber-Sudarshan P function into spherical harmonics and calculate a numerical approximation by randomly sampling a large number of states and mixing them with the fully mixed state until their quantumness vanishes. We start by defining the above concepts more precisely.

II. ABSOLUTELY CLASSICAL STATES

A. Classical spin states

Pure classical spin states were defined in [11] as $SU(2)$ coherent states. This is motivated by the fact that these states have minimal possible uncertainty of the angular momentum operator \mathbf{J} . Moreover, when the spin undergoes a unitary time evolution driven by a Hamiltonian linear in the components of \mathbf{J} , corresponding, for example, to a precession in a magnetic field, this minimal uncertainty property is conserved (similarly as what happens for field coherent states; see, e.g., [24]). A spin- j coherent state points in a well-defined direction \mathbf{n} that we can parametrize with polar and azimuthal angles θ, ϕ as $\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. In terms of the usual $|j, m\rangle$ basis states [i.e., eigenstates of \mathbf{J}^2 and J_z with eigenvalues $j(j+1)$ and m , respectively, with $\hbar = 1$], a spin- j coherent state can be expanded as [25]

$$|\alpha\rangle = \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2} e^{-i\phi}\right)^{j-m} |j, m\rangle, \quad (1)$$

with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi[$. By a stereographic projection $\alpha = e^{i\phi} \tan(\theta/2)$, we can alternatively parametrize the spin- j coherent states with a complex number α . The $|\alpha\rangle$ form an overcomplete basis and we have the identity $(1/4\pi) \int d\alpha |\alpha\rangle\langle\alpha| = I_{2j+1}$, where I_{2j+1} is the identity operator in the $(2j+1)$ -dimensional Hilbert space spanned by the $|j, m\rangle$ basis states. Any density operator ρ of a spin- j state can be expanded in terms of the $|\alpha\rangle$ in the form of a diagonal representation,

$$\rho = \int d\alpha P(\alpha) |\alpha\rangle\langle\alpha|, \quad (2)$$

where $P(\alpha)$ is known as the (Glauber-Sudarshan) P function [26] [in general, $P(\alpha)$ depends on both α and α^* , but it is customary to write $P(\alpha)$ for short].

Classically mixing pure states should not increase their quantumness. This principle underlies the well-known definition of classicality in quantum optics [27]. In close correspondence, one can therefore define mixed classical spin states as those states that can be written as a classical mixture of spin- j coherent states, i.e., a convex combination of projectors onto spin- j coherent states. This means that a general spin- j state ρ is classical iff there exists a positive function $P(\alpha)$ with which ρ can be written as in Eq. (2) [11]. Note that the P function is not unique: indeed, when expanded over spherical harmonics $Y_{KQ}(\theta, \phi)$, only components with $K \leq 2j$ play a

role in the integral (2), so that arbitrary spherical harmonics with $K \geq 2j+1$ can be added to $P(\alpha)$ without changing ρ (see an example in [11]). Classical spin- j states are hence those states for which at least one P function is positive. Classical spin- j states form a convex set by definition.

Deciding whether or not a spin- j state is classical then becomes a problem of convex optimization (see below). Note that the Wigner function of a spin- j coherent state is not everywhere positive in general, not even for a spin $1/2$; see [28].

This is different from the harmonic oscillator, where positivity of the P function implies positivity of W .

B. Absolutely classical spin states

Let \mathcal{H}_m be a Hilbert space of dimension d_m , and $\mathcal{B}(\mathcal{H}_m)$ the space of bounded linear operators on \mathcal{H}_m . Consider a bipartite physical system with Hilbert space $\mathcal{H} = \mathcal{H}_m \otimes \mathcal{H}_n$. In [17], the absolute separability problem was introduced: What are the states $\rho \in \mathcal{B}(\mathcal{H})$ such that $U\rho U^\dagger$ is separable for all unitary matrices $U \in \mathcal{B}(\mathcal{H})$? The problem can also be understood as “separability from spectrum” problem [18]: Since all $U\rho U^\dagger$ have the same spectrum of eigenvalues as ρ , it is natural to try to characterize the set of absolutely separable states by conditions on the spectrum. For $n = m = 2$, a necessary and sufficient condition is known in terms of a single inequality for the eigenvalues [19]: if $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are the eigenvalues of ρ , then it is absolutely separable if and only if $[(\lambda_1 - \lambda_3)^2 + (\lambda_2 - \lambda_4)^2]^{1/2} \leq \lambda_2 + \lambda_4$. Absolute separability is evidently a stronger condition than separability. For instance, a coherent state of two spins $1/2$ is a separable state, but it can become entangled under a general unitary transformation $U \in \mathcal{B}(\mathcal{H})$. More generally, no pure two-qubit state satisfies the above inequality, hence any two-qubit absolutely separable state is mixed. The general problem is still open.

In [20], an important step was made by finding the largest ball of separable states (in terms of any p norm, $0 \leq p \leq \infty$) centered at the maximally mixed state $\rho_0 = I_m \otimes I_n/d$ with $d = mn$. In the Frobenius norm ($p = 2$), its radius is given by $r_d = 1/\sqrt{d(d-1)}$, i.e., all ρ with $\|\rho - \rho_0\| \leq r_d$ are separable, and r_d is the largest such constant. In terms of purity, this means that ρ is separable if the purity $\text{tr}\rho^2$ is less than or equal to $1/(d-1)$, as was already conjectured in [21]. Although all states within this ball are absolutely separable, there are also absolutely separable states outside this ball [22]. This can be clearly seen in the case $n = m = 2$: it is easy to find examples of states ρ whose distance to ρ_0 in the Frobenius norm satisfies $[\sum_i (\lambda_i - 1/4)^2]^{1/2} > r_d = 1/\sqrt{12}$, while the absolute separability condition $[(\lambda_1 - \lambda_3)^2 + (\lambda_2 - \lambda_4)^2]^{1/2} \leq \lambda_2 + \lambda_4$ is satisfied (for instance, $\lambda_1 = \lambda_2 = 13/32$ and $\lambda_3 = \lambda_4 = 3/32$). Witnesses for states that are not absolutely separable were introduced in [23].

Here we ask a corresponding question for classicality: what are the spin- j states $\rho \in \mathcal{B}(\mathcal{H}_{2j+1})$ such that $U\rho U^\dagger$ is classical for all unitary matrices $U \in \mathcal{B}(\mathcal{H}_{2j+1})$? The states that fulfill this criterion will be called “absolutely classical.” They are such that no unitary spin- j operator can create quantumness or, equivalently, entanglement among the underlying $N = 2j$ spins $1/2$. We proceed similarly to the approach of [20], i.e., we establish a lower bound on the maximal radius $r_{\max}(j)$ of the

ball around the maximally mixed state $\rho_0 = I_{2j+1}/(2j+1)$, in which any state is classical.

C. Analytical lower bound for $r_{\max}(j)$

Let ρ be an arbitrary density matrix of a spin- j state. This state can always be written as

$$\rho(r) = \rho_0 + r\tilde{\rho}, \quad (3)$$

where $\rho_0 = I_{2j+1}/(2j+1)$, and $\tilde{\rho} = (\rho - \rho_0)/\|\rho - \rho_0\|$ is traceless and normalized so that the (Hilbert-Schmidt or Frobenius) norm of $\tilde{\rho}$ is $\|\tilde{\rho}\|^2 = \text{tr}\tilde{\rho}^2 = 1$ without restriction of generality. This fixes the scale for the real positive parameter r . Therefore, the state $\rho(r)$ is at the distance r from the maximally mixed state. The P function of $\rho(r)$, defined through the coherent state representation

$$\rho(r) = \int d\alpha P(r, \alpha) |\alpha\rangle\langle\alpha|, \quad (4)$$

can be written

$$P(r, \alpha) = \frac{1}{4\pi} + r\tilde{P}(\alpha), \quad (5)$$

where $1/4\pi$ is the P function of ρ_0 . In order to show that for a given r and arbitrary direction $\tilde{\rho}$ a positive P function can be found, it is enough to consider traceless parts that can be expanded as

$$\tilde{P}(\alpha) = \sum_{K=1}^{2j} \sum_{Q=-K}^K \tilde{P}_{KQ} Y_{KQ}(\alpha), \quad (6)$$

where the Y_{KQ} are spherical harmonics and $\tilde{P}_{KQ} \in \mathbb{C}$. Note that more generally, $\tilde{P}(\alpha)$ can contain spherical harmonics with arbitrarily large K , but any $\rho(r)$ can be represented by a P function that contains values of K only up to $2j$. Indeed, a given quantum state fixes the components in $P(\alpha)$ up to $K = 2j$ uniquely (see below), whereas the higher ones are arbitrary. Hence we can set them to zero and look for the largest r that still guarantees for all $\tilde{\rho}$ a positive $P(\alpha)$ of the form (6). We can expand $\tilde{\rho}$ in terms of the irreducible tensor operators T_{KQ} as

$$\tilde{\rho} = \sum_{K=1}^{2j} \sum_{Q=-K}^K \tilde{\rho}_{KQ} T_{KQ}. \quad (7)$$

Completely analogously, we can also expand $\rho(r)$ and $P(r, \alpha)$ in terms of T_{KQ} and $Y_{KQ}(\alpha)$, respectively,

$$\rho(r) = \sum_{K=0}^{2j} \sum_{Q=-K}^K \rho_{KQ}(r) T_{KQ}, \quad (8)$$

$$P(r, \alpha) = \sum_{K=0}^{2j} \sum_{Q=-K}^K P_{KQ}(r) Y_{KQ}(\alpha). \quad (9)$$

One then immediately finds $P_{KQ}(r) = r\tilde{P}_{KQ}$ and $\rho_{KQ}(r) = r\tilde{\rho}_{KQ}$ for all integer $K \geq 1$ and $-K \leq Q \leq K$. Since $\rho(r)$ is a valid density matrix, the $P_{KQ}(r)$ are related to the $\rho_{KQ}(r)$ by a simple factor [29],

$$P_{KQ}(r) = f_{KQ} \rho_{KQ}(r) \quad \forall K, Q, \quad (10)$$

$$f_{KQ} = (-1)^{K-Q} \frac{\sqrt{(2j-K)!(2j+K+1)!}}{2\sqrt{\pi}(2j)!}, \quad (11)$$

and hence also

$$\tilde{P}_{KQ} = f_{KQ} \tilde{\rho}_{KQ}, \quad (12)$$

$\forall K \geq 1, -K \leq Q \leq K$. The Cauchy-Schwarz inequality applied to (6) then yields

$$|\tilde{P}(\alpha)| \leq \left(\sum_{K=1}^{2j} \sum_{Q=-K}^K |\tilde{\rho}_{KQ}|^2 \right)^{1/2} \times \left(\sum_{K=1}^{2j} \sum_{Q=-K}^K |f_{KQ} Y_{KQ}(\alpha)|^2 \right)^{1/2}. \quad (13)$$

The normalization of $\tilde{\rho}$ implies

$$\begin{aligned} \sum_{K=1}^{2j} \sum_{Q=-K}^K |\tilde{\rho}_{KQ}|^2 &= \sum_{K, K'=1}^{2j} \sum_{Q, Q'=-K}^K \tilde{\rho}_{KQ} \tilde{\rho}_{K'Q'}^* \text{tr} T_{KQ} T_{K'Q'}^\dagger \\ &= \text{tr} \tilde{\rho}^2 = 1, \end{aligned} \quad (14)$$

where we have used the orthogonality of the irreducible tensor operators. By noting that $|f_{KQ}|$ is independent of Q and using the identity

$$\sum_{Q=-K}^K |Y_{KQ}(\theta, \varphi)|^2 = \frac{2K+1}{4\pi}, \quad (15)$$

we get from (13) that $|\tilde{P}(\alpha)| \leq \tilde{P}_{\max}^{(j)}$, with

$$\tilde{P}_{\max}^{(j)} = \left\{ \frac{2j+1}{8\pi^2} \left[(4j+1) \binom{4j}{2j} - (j+1) \right] \right\}^{1/2}. \quad (16)$$

This implies a lower bound $\tilde{P}(\alpha) \geq -\tilde{P}_{\max}^{(j)}$, and hence

$$P(r, \alpha) = \frac{1}{4\pi} + r\tilde{P}(\alpha) \geq \frac{1}{4\pi} - r\tilde{P}_{\max}^{(j)}. \quad (17)$$

If the right-hand side is non-negative, so is the left-hand side. Thus if

$$\begin{aligned} r &\leq \frac{1}{4\pi \tilde{P}_{\max}^{(j)}} = \left\{ (4j+2) \left[(4j+1) \binom{4j}{2j} - (j+1) \right] \right\}^{-1/2} \\ &\equiv \hat{r}_{\max}(j) \end{aligned} \quad (18)$$

in the state (3), then the P function, given by $P(r, \alpha)$ in Eq. (5), is positive. Hence, $\rho(r)$ is classical for $r \leq \hat{r}_{\max}(j)$. Since $\rho(r) = \rho$ for $r = \|\rho - \rho_0\|$, we have proved that

$$\|\rho - \rho_0\| \leq \hat{r}_{\max}(j) \Rightarrow \rho \in \mathcal{C}, \quad (19)$$

where \mathcal{C} is the set of classical states. The distance $\|\rho - \rho_0\|$ is invariant under conjugation by an arbitrary unitary matrix $U \in \mathcal{B}(\mathcal{H}_{2j+1})$. Hence, if ρ satisfies the inequality in (19), all states $U\rho U^\dagger$ verify $\|U\rho U^\dagger - \rho_0\| \leq \hat{r}_{\max}(j)$ and are thus classical. Therefore, $\hat{r}_{\max}(j)$ is a lower bound for the ball size $r_{\max}(j)$.

The Cauchy-Schwarz inequality (13) can be saturated for any given α by choosing $\tilde{\rho}_{KQ} = A f_{KQ} Y_{KQ}(\alpha)$, where A is a proportionality constant such that $\text{tr} \tilde{\rho}^2 = 1$. However, due to the restriction of the P function to (6), with components $K \leq 2j$ only, we do not exhaust all possible P functions. Hence, it may be possible to increase the lower bound of $\tilde{P}(\alpha)$ in (16) by adding components Y_{KQ} with $K > 2j$.

D. Numerical result for $r_{\max}(j)$

To test the lower bound (18), we search for nonclassical states that are as close as possible to the maximally mixed state, since each of these states gives an upper bound on the true ball size $r_{\max}(j)$.

To do this, we generate random mixed states ρ from the Hilbert-Schmidt ensemble of matrices $\rho = AA^\dagger/\text{tr}(AA^\dagger)$, with A a complex matrix with independent Gaussian entries (see [30] for details). With these states, we construct families of states,

$$\rho_k = (1 - k)\rho_0 + k\rho, \quad (20)$$

as function of a parameter $k \in [0,1]$, which interpolate between the maximally mixed state ρ_0 and the state ρ . The task is to find the largest value k_{\max} of k , under the condition that ρ_k is classical. This can be rewritten as

$$\max_k k \quad \text{such that} \quad \rho_k = \int d\alpha P(\alpha)|\alpha\rangle\langle\alpha|, P(\alpha) \geq 0. \quad (21)$$

This problem can be formulated in the form of a linear programming problem, of the form

$$\max_x c^T x \quad \text{such that} \quad Ax = b, x \geq 0, \quad (22)$$

where x is the vector of variables, c, b are real given vectors, and A is a real given matrix. These types of optimizations can be solved very efficiently, e.g., with an interior-point method [31]. Another great property is the existence of a dual problem. If the optimal value of the dual problem coincides with the optimal value of the original problem (22), i.e., if there is no duality gap, the solution is proven to be optimal. We will now explain how to reformulate the problem (21) in the form (22).

Due to Carathéodory's theorem, a positive P function for finite j can always be written as a convex sum of δ functions, so any classical state has the form $\sum_{i=1}^N w_i |\alpha_i\rangle\langle\alpha_i|$ with $w_i \geq 0$ and $N \leq (2j + 1)^2$ (where the number of states needed is reduced by one due to normalization of the state). With this form, ρ_k is classical iff there exist $w_i \geq 0$ with $\sum_i w_i = 1$ and coherent states $|\alpha_i\rangle$ such that

$$\sum_{i=1}^N w_i |\alpha_i\rangle\langle\alpha_i| = \rho_k, \quad (23)$$

which can be rewritten as

$$\sum_{i=1}^N w_i |\alpha_i\rangle\langle\alpha_i| + k(\rho_0 - \rho) = \rho_0. \quad (24)$$

This equation can be written as $Ax = b$ as in (22), where the vector of variables is given by $x = (\{w_i\}_{i=1,\dots,N}, k)$. The vector b is fixed by the maximally mixed state, and the matrix A is constructed from the real and imaginary entries of the left-hand side of Eq. (24). Then with the choice $c = (0, \dots, 0, 1)$ in (22), the problem (21) is in the form of a linear optimization problem.

However, since the α_i in (24) are unknown, we generate a large list of uniformly distributed coherent states, of the order of 10^6 many, so that it should be possible to construct almost all classical states by varying the weights w_i . This assumption can be tested by repeating the linear optimization with a new

set of random angles and also with an increased number of them. These tests showed that for $j \leq 21/2$, increasing the number of random angles beyond 10^6 does not visibly change the results.

We applied this procedure to a list of $n \sim 3000$ different states ρ in (20) for system sizes of up to $j = 21/2$. The states that maximize k are found at distances

$$r_l = \|\rho_{\tilde{k}_{\max}} - \rho_0\| = \|\rho - \rho_0\| \tilde{k}_{\max}, \quad l = 1, 2, \dots, n, \quad (25)$$

from the fully mixed spin- j state, where \tilde{k}_{\max} is the numerical result of the optimization problem (22) and (24). Numerically, not all directions ρ can be sampled, and only a finite number of coherent states can be considered. On the one hand, the fact that we can sample only a finite number of coherent states entails that the numerically found \tilde{k}_{\max} for a given ρ is a lower bound of the corresponding exact k_{\max} . On the other hand, even if one started with all coherent states, as in the decomposition (21), one would achieve the exact values $\tilde{k}_{\max} = k_{\max}$, but each r_l , and hence $\tilde{r}_{\max}(j) \equiv \min_{1 \leq l \leq n} r_l$, would still give only an upper bound on the true radius of the ball $r_{\max}(j)$. Therefore, \tilde{r}_{\max} is simply a numerical approximation of r_{\max} , but *a priori* neither a strict upper nor lower bound.

It is worth mentioning that the entangled states closest to the maximally mixed state are not on a straight line with the queen of quantum state, i.e., the state with maximum quantumness for given j [15], except in the $j = 1$ case.

III. DISCUSSION

In Fig. 1, we compare the numerically found $\tilde{r}_{\max}(j)$ and the analytical lower bound $\hat{r}_{\max}(j)$ from Eq. (18) with the radius of the ball of absolutely separable states, $r_d = 1/(2^j \sqrt{4^j - 1})$ with $d = 2^{2j}$ [20]. The lower bound $\hat{r}_{\max}(j)$ decays exponentially with j . It is still substantially below the numerically found $\tilde{r}_{\max}(j)$, which can be considered close to the exact value $r_{\max}(j)$. Also, $\tilde{r}_{\max}(j)$ decays exponentially

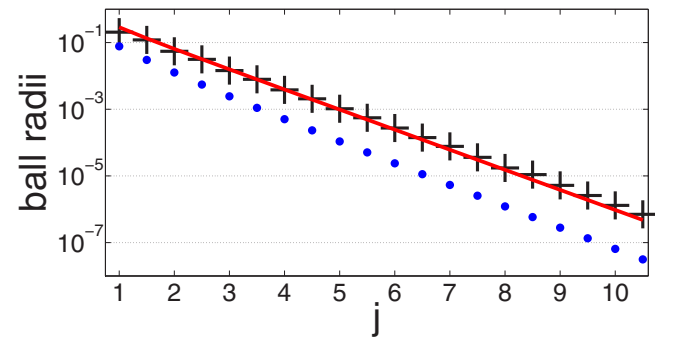


FIG. 1. Maximal radius $r_{\max}(j)$ of a ball of classical states centered at the fully mixed state as a function of j . Blue dots: the value of the lower bound $\hat{r}_{\max}(j)$; Eq. (18). Black crosses: smallest numerically found distance from the maximally mixed state to a nonclassical state. Red line: maximal ball size $1/(2^j \sqrt{4^j - 1})$ for arbitrary (not necessarily symmetric) separable states [20]. This function gives an excellent approximation of the numerically found maximal ball size $\tilde{r}_{\max}(j)$ of classical spin- j states, but slightly overestimates it for small j .

with j , and the ratio between $\tilde{r}_{\max}(j)$ and $\hat{r}_{\max}(j)$ increases only slowly with increasing j over the whole examined range $1 \leq j \leq 10.5$. The function $1/(2^j \sqrt{4^j - 1})$ agrees with $\tilde{r}_{\max}(j)$ remarkably well over the whole range of ρ . However, it is not to be expected that $1/(2^j \sqrt{4^j - 1})$ is the correct result for $r_{\max}(j)$ for at least two reasons: (i) The fully mixed state in the fully symmetric sector of Hilbert space $I_{2^{j+1}}/(2j+1)$ (under exchange of qubits) is not identical to the fully mixed state in the full Hilbert space \mathcal{H} , $I_{2^{2j}}/2^{2j}$, of $N = 2j$ spins $1/2$. Hence, the balls of absolutely separable states and absolutely classical states are not centered at the same point. For example, for two spins $1/2$, we have a fully symmetric subspace of \mathcal{H} of dimension 3 (the triplet sector) with the identity matrix $I_3 \equiv \sum_{m=-1}^1 |1, m\rangle\langle 1, m|$, whereas the identity in the full \mathcal{H} also contains a projector onto the singlet state $|j = 0, m = 0\rangle\langle j = 0, m = 0|$, and has hence to be normalized differently as well, $I_4 \equiv \sum_{j=0,1} \sum_{m=-j}^j |j, m\rangle\langle j, m|$. (ii) When minimizing the distance to nonclassical states, the relevant set of states is larger without the restriction to symmetric states. From the latter argument, one would expect that $1/(2^j \sqrt{4^j - 1})$ underestimated $r_{\max}(j)$, if it were evaluated centered on the same identity. This appears to be correct for large values of j

(starting at about $j \geq 4$), but could also be due to the numerical uncertainty of the very small value of $r_{\max}(j)$. For small values of j , we have rather $\tilde{r}_{\max}(j) < 1/(2^j \sqrt{4^j - 1})$. The case $j = 1$ is particularly instructive, as there we have a full analytical characterization of the set of classical states [13]. The numerically found value $\tilde{r}_{\max}(j) \simeq 0.2052$ agrees well with the analytical one $1/(2\sqrt{6}) \simeq 0.2041$, whereas $1/(2^j \sqrt{4^j - 1}) = 1/(2\sqrt{3}) \simeq 0.288$. Nevertheless, altogether we see that the closest nonclassical symmetric state of a spin j is about as close to the fully mixed state in the symmetric sector as the closest entangled state without any symmetry restrictions to the fully mixed state in the full 2^{2j} -dimensional Hilbert space of $N = 2j$ spins $1/2$.

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A.5. Regularly Decomposable Tensors and Classical Spin States

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Regularly Decomposable Tensors and Classical Spin States ^{*}

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Abstract

Recently, in physics, a tensor representation for spin states was introduced. The tensor representing a spin- j state is a symmetric tensor of order $N = 2j$ and dimension 4. Here, j can be a positive integer, which corresponds to a boson; j can also be a positive half-integer, which corresponds to a fermion. In this paper, we introduce regularly decomposable tensors. In the even-order case, a regularly decomposable tensor is a completely decomposable tensor but not vice versa; a completely decomposable tensor is a sum-of-squares (SOS) tensor but not vice versa; an SOS tensor is a positive semi-definite (PSD) tensor but not vice versa. In the odd-order case, the first row tensor of a regularly decomposable tensor is regularly decomposable and its other row tensors are induced by the regular decomposition of its first row tensor. In the literature, PSD and SOS tensors have been studied extensively, but very little has been studied for completely decomposable tensors, and regularly decomposable tensors are only introduced here. We show that in both the odd-order (fermion) and even-order (boson) cases a spin- j state is classical if and only if its representing tensor is a regularly decomposable tensor. Complete decomposability and regular decomposability are invariant under orthogonal transformations of the tensor. We also show that the completely decomposable tensor cone and the regularly decomposable tensor cone are closed convex cones. Furthermore, in the even-order case, the completely decomposable tensor cone and the PSD tensor cone are dual to each other. The Hadamard product of two completely decomposable tensors is still a completely decomposable tensor. Since one may apply the positive semi-definite programming algorithm to detect whether a symmetric tensor is an SOS tensor or not, this gives a checkable necessary condition for classicality of a spin- j state. Further research issues on regularly decomposable tensors are also raised.

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1 Introduction

A geometrical picture of quantum states often helps getting some insight on underlying physical properties. For arbitrary pure spin states, such a geometrical representation was developed by Ettore Majorana [1]: a spin- j state is visualized as $N = 2j$ points on the unit sphere S^2 , called in this context the Bloch sphere. The advantage of such a picture is a direct interpretation of certain unitary operations: namely, if a quantum spin- j state is mapped to another one by a unitary operation that correspond to a $(2j + 1)$ -dimensional representation of a spatial rotation, its Majorana points are mapped to points obtained by that spatial rotation. Recently a tensor representation of an arbitrary mixed or pure spin- j state was proposed that generalizes this picture [2]. It consists of a real symmetric tensor of order $N = 2j$ and dimension 4. A spin- j state corresponds to a boson if j is a positive integer, and corresponds to a fermion if j is a positive half-integer. Thus, a boson corresponds to an even-order four dimensional tensor, while a fermion corresponds to an odd order four dimensional tensor.

The geometrical picture is particularly useful when it comes to studying classicality properties of spin states. In quantum optics, coherent states are quantum states that behave the most classically, in that they minimize the uncertainty relation between position and momentum. Coherent states can also be defined in the context of spins. Statistical mixtures of coherent states can thus be considered the “least quantum” states. The set of classical spin states was introduced in [3] as the convex hull of the set of coherent spin states. It can be interpreted (see e.g. [4]) as the set of fully separable states in the symmetric sector of the tensor product of $2j$ spins-1/2. The above geometric picture easily allows one to characterize coherent spin states: a coherent spin- j state can be represented by $N = 2j$ points located at the same position on the Bloch sphere. The characterization of classical states is less easy to obtain, but the tensorial picture helps to get some results on this issue. For instance, in [4] it was shown that when j is an integer, i.e., N is an even number, a classical spin- j state is such that its representing tensor is positive semi-definite (PSD) in the sense of [5] (see Section 2).

Positive semi-definiteness of the tensor representation is a necessary and sufficient condition of classicality in the case $j = 1$ [6]. It is only a necessary condition for classicality of a spin- j state, and only if j is a positive integer, as pointed out in [4]. A natural question is therefore whether it is possible to formulate a necessary and sufficient condition for classicality of a spin- j state in terms of its tensor representation, first in the case where j is a positive integer, i.e., the boson case, and then in the case where j is a half-integer, i.e., the fermion case. The aim of this paper is to introduce tools in order to reformulate these two questions from a mathematical perspective.

The PSD condition can be expressed in terms of tensor eigenvalues. A tensor is PSD if and only if its smallest H-eigenvalue or Z-eigenvalue is nonnegative [5]. This links classicality of a spin- j state (with j as a positive integer) with the smallest tensor eigenvalue of its representing tensor. This result echoes the result of [7], which stated that the geometric measure of entanglement of a pure state is equal to the largest tensor eigenvalue. Note that tensor eigenvalues have found applications in different areas of physics [8, 9, 10, 11]. To go beyond the PSD condition for classicality, we have to consider stronger properties. A property stronger than positive semi-definiteness is the sum-of-squares (SOS) property. SOS tensors were introduced in [12, 13]. According to the Hilbert theory [14], an SOS tensor is a PSD tensor but not vice versa. Both PSD and SOS tensors have been studied intensively in recent years. Some references on PSD and SOS tensors include [15, 16, 17, 18, 19, 20, 21, 22]. One can show

(see below) that when j is an integer, if a spin- j state is classical, then its representing tensor is an SOS tensor in the sense of [15, 12, 13]. But this is still a necessary condition. A property stronger than the SOS property is complete decomposability. Completely decomposable tensors were introduced and studied in [23, 24]. An even-order completely decomposable tensor is an SOS tensor but not vice versa [23, 24]. Again, when j is an integer, if a spin- j state is classical, then its representing tensor is a completely decomposable tensor, and this is still a necessary condition.

In this paper, we introduce regularly decomposable tensors. A regularly decomposable tensor is a completely decomposable tensor but not vice versa. Furthermore, we define regularly decomposable tensors also in the odd-order case. In the odd-order case, the first row tensor of a regularly decomposable tensor is regularly decomposable and its other row tensors are induced by the regular decomposition of its first row tensor. We show that in both the odd-order (fermion) and even-order (boson) cases a spin- j state is classical if and only if its representing tensor is a regularly decomposable tensor. Thus, it is important to study properties of regularly decomposable tensors and completely decomposable tensors, as well as some further properties of PSD tensors and SOS tensors.

The remaining part of this paper is organized as follows. In Section 2, we review the definitions of PSD, SOS and completely decomposable tensors, and define regularly decomposable tensors. In Section 3, we show that in both the odd-order (fermion) and even-order (boson) cases a spin- j state is classical if and only if its representing tensor is a regularly decomposable tensor. Some properties of completely decomposable tensors and regularly decomposable tensors and their implications in physics are studied in Section 4. Some further research issues on regularly decomposable tensors are raised in Section 5.

2 PSD, SOS, Completely Decomposable and Regularly Decomposable Tensors

In this paper, for a vector $\mathbf{x} \in \mathfrak{R}^{n+1}$, we denote it as $\mathbf{x} = (x_0, x_1, \dots, x_n)^\top$. Later, in physical applications, we will have $n = 3$. Here, we assume that $n \geq 2$. Denote the zero vector in \mathfrak{R}^{n+1} by $\mathbf{0}$.

Let $\mathcal{A} = (a_{i_1 \dots i_m})$ be an m th order $(n+1)$ -dimensional real tensor. We say that \mathcal{A} is a symmetric tensor if the entries $a_{i_1 \dots i_m}$ are invariant under permutation of their indices. Denote $T_{m,n+1}$ as the set of all m th order $(n+1)$ -dimensional real tensors, and $S_{m,n+1}$ as the set of all m th order $(n+1)$ -dimensional real symmetric tensors. Then $T_{m,n+1}$ is a linear space, and $S_{m,n+1}$ is a linear subspace of $T_{m,n+1}$. Denote the zero tensor in $S_{m,n+1}$ by \mathcal{O} .

Let $\mathcal{A} = (a_{i_1 \dots i_m}) \in T_{m,n+1}$ and $\mathcal{B} = (b_{i_1 \dots i_p}) \in T_{p,n+1}$. The outer product of \mathcal{A} and \mathcal{B} , denoted as $\mathcal{C} = \mathcal{A} \otimes \mathcal{B}$, is a real tensor in $T_{m+p,n+1}$, defined by $\mathcal{C} = (a_{i_1 \dots i_m} b_{i_{m+1} \dots i_{m+p}})$. We also denote $\mathcal{A}^{\otimes 2} = \mathcal{A} \otimes \mathcal{A}$, $\mathcal{A}^{\otimes (k+1)} = \mathcal{A}^{\otimes k} \otimes \mathcal{A}$ for $k \geq 2$. A *symmetric rank-one* tensor is defined as a symmetric tensor in $S_{m,n+1}$ of the form $\alpha \mathbf{x}^{\otimes m}$, where $\alpha \in \mathfrak{R}$ and $\mathbf{x} \in \mathfrak{R}^{n+1}$.

Let $\mathcal{A} = (a_{i_1 \dots i_m})$ and $\mathcal{B} = (b_{i_1 \dots i_m})$ in $S_{m,n+1}$. The inner product of \mathcal{A} and \mathcal{B} , denoted as $\mathcal{A} \bullet \mathcal{B}$, is a scalar, defined by

$$\mathcal{A} \bullet \mathcal{B} = \sum_{i_1, \dots, i_m=0}^n a_{i_1 \dots i_m} b_{i_1 \dots i_m}.$$

Let $\mathcal{A} = (a_{i_1 \dots i_m}) \in S_{m,n+1}$ and $\mathbf{x} \in \mathfrak{R}^{n+1}$. Then we have

$$\mathcal{A} \bullet \mathbf{x}^{\otimes m} \equiv \sum_{i_1, \dots, i_m=0}^n a_{i_1 \dots i_m} x_{i_1} \dots x_{i_m}.$$

If for any $\mathbf{x} \in \mathfrak{R}^{n+1}$, we have $\mathcal{A} \bullet \mathbf{x}^{\otimes m} \geq 0$, then we say that \mathcal{A} is a **positive semi-definite (PSD)** tensor. If for any $\mathbf{x} \in \mathfrak{R}^{n+1}$, $\mathbf{x} \neq \mathbf{0}$, we have $\mathcal{A} \bullet \mathbf{x}^{\otimes m} > 0$, then we say that \mathcal{A} is a **positive definite**

(PD) tensor. Clearly, if m is odd, then the only PSD tensor is the zero tensor, and there is no PD tensor. Thus, we only discuss even-order PSD and PD tensors.

Suppose that $m = 2l$ is even. Let $\mathcal{A} \in S_{m,n+1}$. If there are symmetric tensors $\mathcal{A}^{(1)}, \dots, \mathcal{A}^{(r)} \in S_{l,n+1}$ such that for all $\mathbf{x} \in \mathfrak{R}^{n+1}$,

$$\mathcal{A} \bullet \mathbf{x}^{\otimes m} = \sum_{k=1}^r \left(\mathcal{A}^{(k)} \bullet \mathbf{x}^{\otimes l} \right)^2,$$

then \mathcal{A} is called a **sum-of-squares (SOS)** tensor. Then, for any $\mathbf{x} \in \mathfrak{R}^{n+1}$, we have $\mathcal{A} \bullet \mathbf{x}^{\otimes m} \geq 0$. Thus, an SOS tensor is always a PSD tensor, but not vice versa. By the Hilbert theory [14], only in the following three cases: 1) $m = 2$, 2) $n = 1$, 3) $m = 4$ and $n = 2$, a PSD tensor is always an SOS tensor; otherwise, there are always PSD tensors which are not SOS tensors. David Hilbert [14] stated this in the language of polynomials. But the meanings are the same.

Let $\mathcal{A} \in S_{m,n+1}$. Here, m can be either even or odd. If there are vectors $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)} \in \mathfrak{R}^{n+1}$ such that

$$\mathcal{A} = \sum_{k=1}^r \left(\mathbf{u}^{(k)} \right)^{\otimes m}, \quad (2.1)$$

then we say that \mathcal{A} is a **completely decomposable tensor**. If all the vectors $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)} \in \mathfrak{R}^{n+1}$ are nonnegative vectors, then \mathcal{A} is called a **completely positive** tensor [34, 20]. Actually, all odd-order symmetric tensors are completely decomposable tensors [23]. Thus, the concept of completely decomposable tensors is not useful for odd order. However, if $m = 2l$ is even, and \mathcal{A} is a completely decomposable tensor as defined by (2.1), then by letting $\mathcal{A}^{(k)} = \left(\mathbf{u}^{(k)} \right)^{\otimes l}$, we see that \mathcal{A} is an SOS tensor. On the other hand, by the examples given in [23, 24], an SOS tensor may not be a completely decomposable tensor.

In order to define regularly decomposable tensors, we still need two more concepts: regular vectors and row-tensors.

Definition 2.1 Let $\mathbf{x} = (x_0, x_1, \dots, x_n)^\top \in \mathfrak{R}^{n+1}$. We say that \mathbf{x} is a **regular vector** if $x_0 \neq 0$ and $x_0^2 = x_1^2 + \dots + x_n^2$.

Definition 2.2 For any $\mathcal{A} = (a_{i_1 \dots i_m}) \in S_{m,n+1}$, define its i th **row tensor** \mathcal{A}_i as a symmetric tensor in $S_{m-1,n+1}$, by $\mathcal{A}_i = (a_{i i_2 \dots i_m})$, for $i = 0, \dots, n$.

We can then define regularly decomposable tensors as follows:

Definition 2.3 (i.) Let the order $m = 2l$ be even and $\mathcal{A} \in S_{m,n+1}$. If \mathcal{A} is a completely decomposable tensor defined by (2.1), where $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)}$ are regular vectors, then we say that \mathcal{A} is a **regularly decomposable tensor** of even order.

(ii.) Let the order $m = 2l + 1$ be odd and $\mathcal{A} \in S_{m,n+1}$. If $\mathcal{A}_0 \in S_{2l,n+1}$ is a regularly decomposable tensor with the regular decomposition

$$\mathcal{A}_0 = \sum_{k=1}^r \left(\mathbf{u}^{(k)} \right)^{\otimes 2l}, \quad (2.2)$$

where $\mathbf{u}^{(k)} = \left(u_0^{(k)}, \dots, u_n^{(k)} \right)^\top$, $k = 1, \dots, r$, are regular vectors, and the other row tensors of \mathcal{A} are induced by this regular decomposition,

$$\mathcal{A}_i = \sum_{k=1}^r \frac{u_i^{(k)}}{u_0^{(k)}} \left(\mathbf{u}^{(k)} \right)^{\otimes 2l}, \quad (2.3)$$

for $i = 1, \dots, n$, then we say that \mathcal{A} is a **regularly decomposable tensor** of odd order.

Clearly an even-order regularly decomposable tensor is a completely decomposable tensor but not vice versa.

Theorem 2.4 *A regularly decomposable tensor $\mathcal{A} = (a_{i_1 \dots i_m}) \in S_{m, n+1}$ can be written as*

$$\mathcal{A} = \sum_{k=1}^r \alpha_k \left(\mathbf{v}^{(k)} \right)^{\otimes m}, \quad (2.4)$$

where $\alpha_k > 0$ and $\mathbf{v}^{(k)} = \left(1, v_1^{(k)}, \dots, v_n^{(k)} \right)^\top$,

$$\sum_{i=1}^n \left(v_i^{(k)} \right)^2 = 1, \quad (2.5)$$

for $k = 1, \dots, r$. Furthermore, we have

$$a_{00i_3 \dots i_m} = \sum_{i=1}^n a_{ii i_3 \dots i_m} \quad (2.6)$$

for $m \geq 2$ and all $i_3, \dots, i_m = 0, 1, \dots, n$.

Proof. Suppose that m is even, and \mathcal{A} is defined by (2.1), where $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)}$ are regular vectors. Let

$$\mathbf{v}^{(k)} = \frac{\mathbf{u}^{(k)}}{u_0^{(k)}}, \quad (2.7)$$

for $k = 1, \dots, r$. Then we see that \mathcal{A} can be expressed by (2.4), where $\alpha_k = \left(u_0^{(k)} \right)^m > 0$ and $\mathbf{v}^{(k)} = \left(1, v_1^{(k)}, \dots, v_n^{(k)} \right)^\top$ satisfy (2.5) for $k = 1, \dots, r$. Suppose that $m = 2l + 1$ is odd, and \mathcal{A}_0 is defined by (2.2), where $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)}$ are regular vectors and the other row tensors of \mathcal{A} are defined by (2.3). Then we see that \mathcal{A} can also be expressed by (2.4), where $\alpha_k = \left(u_0^{(k)} \right)^{2l} > 0$, $\mathbf{v}^{(k)} = \left(1, v_1^{(k)}, \dots, v_n^{(k)} \right)^\top$, still defined by (2.7), satisfy (2.5) for $k = 1, \dots, r$. By these, we see that (2.6) is satisfied. \square

Suppose that $\mathcal{A} = (a_{i_1 \dots i_m}) \in S_{m, n+1}$ satisfies (2.6). Then we call \mathcal{A} a **regular symmetric tensor**. If moreover $a_{00 \dots 0} = 1$ we call \mathcal{A} a **regular normalized symmetric tensor**. In the next section we will see that an important research issue is to determine whether a given regular symmetric tensor is a regularly decomposable tensor or not.

3 Regularly Decomposable Tensors and Classicality of Spin States

Several definitions of classicality of a quantum state exist in the literature, based e.g. on the positivity of the Wigner function, or the absence of entanglement in the case of multi-partite systems [25, 26, 27, 7, 28]. In [3] a suitable definition of classicality of spin states was introduced. Firstly, pure classical spin states are defined as angular-momentum coherent states, also called ‘‘SU(2)-coherent states’’, and in the following also simply ‘‘coherent states’’. Their properties are well-known from work in quantum optics [29, 30] and quantum-chaos [31]. For being self-contained, we briefly review

them here.

SU(2)-coherent states can be labeled by a complex label α , related by stereographic projection to polar and azimuthal angles θ and ϕ , $\alpha = \tan(\theta/2)e^{i\phi}$. Let $\mathbf{J} \equiv (J_x, J_y, J_z)$ denote the angular momentum vector, and $|j, m\rangle$ the joint-eigenbasis states of the angular momentum component J_z and the total angular momentum $\mathbf{J}^2 \equiv J_x^2 + J_y^2 + J_z^2$, with $J_z |j, m\rangle = m |j, m\rangle$, $\mathbf{J}^2 |j, m\rangle = j(j+1) |j, m\rangle$. The components J_x and J_y are related to the ladder operators J_{\pm} by $J_{\pm} = J_x \pm iJ_y$ and $J_{\pm} |j, m\rangle = \sqrt{j(j+1) - m(m \pm 1)} |j, m \pm 1\rangle$, where $i = \sqrt{-1}$ is the imaginary unit. The coherent states can be written as

$$|\alpha\rangle = \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2} e^{i\phi}\right)^{j-m} |j, m\rangle, \quad (3.8)$$

with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi[$. For $\theta = 0$ or $\theta = \pi$, $|\alpha\rangle = |j, j\rangle$ or $|j, -j\rangle$ respectively, i.e. the angular momentum states with largest or smallest J_z -component are always coherent states. Geometrically, a coherent state $|\alpha\rangle$ with $\alpha = \tan(\theta/2)e^{i\phi}$ is associated to a direction $\hat{\mathbf{n}} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ on the Bloch sphere. Coherent states have the important property that the quantum uncertainty of the rescaled angular momentum vector \mathbf{J}/j of a spin- j is minimal for all pure quantum states, $(\langle \alpha | \mathbf{J}^2 | \alpha \rangle - \langle \alpha | \mathbf{J} | \alpha \rangle^2) / j^2 = 1/j$. The uncertainty vanishes in the classical limit of a large spin, $j \rightarrow \infty$. The coherent states come as closely as possible to the ideal of a classical phase space point, i.e. represent as best as allowed by the laws of quantum mechanics an angular momentum pointing in a precise direction,

$$\langle \alpha | \mathbf{J} | \alpha \rangle = j(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) = j\hat{\mathbf{n}}. \quad (3.9)$$

Another important feature of coherent states is that they remain coherent under unitary transformations of the form $U = e^{-i\gamma \hat{\mathbf{n}} \cdot \mathbf{J}}$. Such unitary transformations arise from the dynamics of the angular momentum in a magnetic field (assuming that the angular momentum is associated with a magnetic moment). Classically, the spin precesses around the axis given by the magnetic field, and this is reproduced by the behavior of the coherent state. One can see this most easily for $\hat{\mathbf{n}} = \hat{e}_z = (0, 0, 1)$, i.e. a magnetic field in the z -direction, in which case $U = e^{-i\gamma J_z}$ can be immediately applied to the basis states $|j, m\rangle$ and gives rise to additional phase factors $e^{-i\gamma m}$, i.e. $\phi \mapsto \phi + \gamma$, and correspondingly the expectation value $\langle \alpha | \mathbf{J} | \alpha \rangle$ is rotated by the angle γ about the z -axis. In general, the mapping $|\alpha\rangle \mapsto |\tilde{\alpha}\rangle = e^{-i\gamma \hat{\mathbf{n}} \cdot \mathbf{J}} |\alpha\rangle$ leads to an expectation value $\langle \tilde{\alpha} | \mathbf{J} | \tilde{\alpha} \rangle = R(\hat{\mathbf{n}}, \gamma) \langle \alpha | \mathbf{J} | \alpha \rangle$, where $R(\hat{\mathbf{n}}, \gamma)$ is a 3×3 orthonormal matrix representing rotation about the axis $\hat{\mathbf{n}}$ with a rotation angle γ . Due to Eq. (3.9), it is clear that all coherent states can be obtained by an appropriate unitary transformation of the form $U = e^{-i\gamma \hat{\mathbf{n}} \cdot \mathbf{J}}$ acting on the state $|j, j\rangle$ associated with the direction \hat{e}_z .

The quantum state of any physical system with finite dimensional Hilbert space can be represented by a density operator (also called density matrix) ρ , a positive semi-definite hermitian operator with $\text{tr} \rho = 1$. If λ_i and $|\psi_i\rangle$ are respectively the eigenvalues and eigenvectors of ρ , one has the eigendecomposition $\rho = \sum_i \lambda_i |\psi_i\rangle \langle \psi_i|$. The density matrix ρ can therefore be interpreted as representing a quantum state which is in some pure state $|\psi_i\rangle$ with probability λ_i . The condition $\text{tr} \rho = 1$ ensures that the probabilities are normalized to 1; it is however possible to work with unnormalized density matrices by relaxing the constraint on $\text{tr} \rho$. In the present paper we will follow that option. As most equations we consider are linear in ρ , this just means that we may forget about an overall normalization constant.

The density operator of an arbitrary spin- j quantum state can be written in the form of a diagonal

representation,

$$\rho = \int_{S^2} d\alpha P(\alpha) |\alpha\rangle\langle\alpha|, \quad (3.10)$$

where $P(\alpha)$ is known as the (Glauber-Sudarshan) P -function [30], and $d\alpha = \sin\theta d\theta d\phi$ is the integration measure over the unit sphere S^2 in three dimensions. Classically mixing states, i.e. drawing randomly pure states according to a classical probability distribution, should not increase the non-classicality of a state. Hence, a spin-state is called classical, if and only if a decomposition of ρ in the form of Eq. (3.10) exists with $P(\alpha) \geq 0$, in which case $P(\alpha)$ can be interpreted as classical probability density of finding the pure SU(2)-coherent state $|\alpha\rangle$ in the mixture. Since by definition classical states form a convex set, Caratheodory's theorem implies immediately that a classical state can be written as a finite convex sum of projectors onto coherent states,

$$\rho = \sum_{i=1}^{(N+1)^2+1} w_i |\alpha_i\rangle\langle\alpha_i|, \quad (3.11)$$

where $w_i \geq 0$. Eq. (3.11) is the general definition of a classical spin state adopted in [3], and we will base the rest of the paper on it.

A single spin-1/2 is equivalent to a qubit, i.e. a quantum-mechanical two state system. The two states “spin-up” and “spin-down”, namely $|\frac{1}{2}, \frac{1}{2}\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle$ in the above $|j, m\rangle$ notation, are also called “computational-basis”. Denoted as $|0\rangle$ and $|1\rangle$ in quantum-information theory, they are represented as column-vectors $(1, 0)^T$ and $(0, 1)^T$. In this basis, the density operator can be represented by a 2×2 complex hermitian matrix with $\text{tr}\rho = 1$ that can be expanded over the Pauli-matrix basis,

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\rho = \frac{1}{2} \sum_{i=0}^3 \sigma_i a_i. \quad (3.12)$$

The four components a_i , $i \in \{0, 1, 2, 3\}$ form an order-1 tensor \mathcal{A} of dimension 4. The Pauli matrices $(\sigma_1, \sigma_2, \sigma_3) \equiv \boldsymbol{\sigma}$ are matrix representations of the components of the operator $2\mathbf{J}$ in the “spin-up” and “spin-down” computational-basis. We have $\text{tr}\rho = a_0$. The vector $\mathbf{v} \equiv (a_1, a_2, a_3)^T \in \mathbb{R}^3$ is the so-called Bloch vector. It satisfies $\|\mathbf{v}\|_2 \leq a_0$ in order to guarantee the positivity of ρ . In particular, $\|\mathbf{v}\|_2 = a_0$ signals pure states (i.e. rank-1 states), and $\|\mathbf{v}\|_2 < a_0$ mixed states (rank-2 states). Due to the orthonormality of the Pauli-matrix basis, \mathbf{v} can be obtained from a given state as $\mathbf{v} = \text{tr}\rho\boldsymbol{\sigma}$. In particular, for a SU(2)-coherent state $|\alpha\rangle$, one finds $\mathbf{v} = \langle\alpha|2\mathbf{J}|\alpha\rangle = (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$, as evidenced by Eq. (3.9). The Bloch picture is particularly useful for visualizing unitary operations: Due to the rotation properties of the coherent states under a unitary operation, if $\tilde{\rho} = U\rho U^\dagger$, the corresponding Bloch vector $\tilde{\mathbf{v}}$ of $\tilde{\rho}$ is obtained by rotation of the original Bloch vector, namely $\tilde{\mathbf{v}} = R(\hat{\mathbf{n}}, \gamma)\mathbf{v}$. As the zero-component of tensor \mathcal{A} has to remain unchanged due to the conservation of the trace under unitary operations, $\tilde{a}_0 = a_0$, the transformation of \mathcal{A} reads $\tilde{a}_i = \mathcal{R}_{ij}a_j$ with

$$\mathcal{R}_{00} = 1, \quad \mathcal{R}_{0i} = \mathcal{R}_{i0} = 0 \quad (i \in \{1, 2, 3\}) \quad \text{and} \quad \mathcal{R}_{ij} = R(\hat{\mathbf{n}}, \gamma)_{ij} \quad (i, j \in \{1, 2, 3\}). \quad (3.13)$$

In [2] the Bloch-vector of a spin-1/2 was generalized to a Bloch-tensor of a spin- j . A spin- j can be composed from $N = 2j$ spins-1/2. The total spin is then the sum of the N spins-1/2, i.e. $\mathbf{J} = \sum_{i=1}^N \boldsymbol{\sigma}^{(i)}/2$. In general, combining two spins j_1 and j_2 gives rise to total spins j ranging from $|j_1 - j_2|$ to $j_1 + j_2$. A spin $j = N/2$ is hence the maximum total spin achievable with N spins-1/2. All basis

states $|j, m\rangle$ can be created by acting with the ladder operator J_- on the state $|j, j\rangle$, which in turn is the state $|\frac{1}{2}, \frac{1}{2}\rangle^{\otimes N}$ of all spins-up in the full Hilbert space of N spins-1/2. Since both $|j, j\rangle$ and J_- are fully symmetric under the exchange of all spins-1/2, all $|j, m\rangle$ states lie in the fully symmetric subspace \mathcal{H}_S of the total Hilbert-space $\mathcal{H} = \mathbb{C}^{2^N}$. A projector \mathcal{P}_S onto that subspace can be obtained as

$$\mathcal{P}_S \equiv \sum_{k=0}^N \left| D_N^{(k)} \right\rangle \left\langle D_N^{(k)} \right|, \quad (3.14)$$

where the so-called Dicke states $|D_N^{(k)}\rangle$ are defined as

$$\left| D_N^{(k)} \right\rangle = \mathcal{N} \sum_{\pi} \underbrace{|0 \dots 0\rangle}_k \underbrace{|1 \dots 1\rangle}_{N-k}, \quad k = 0, \dots, N,$$

\mathcal{N} is a normalization constant, and the sum is over all permutations of the spin-1/2 states, written here as tensor product of the computational basis states $|0\rangle$ and $|1\rangle$ of each spin-1/2. The Dicke states are in 1-1 correspondence with the $|j, m\rangle$ states, with $j = N/2$ and $m = k - N/2$.

It was shown in [2] that a tight frame of matrices $S_{i_1 \dots i_N}$ can be obtained by projecting $\sigma_{i_1 i_2 \dots i_N} \equiv \sigma_{i_1} \otimes \sigma_{i_2} \dots \otimes \sigma_{i_N}$ into \mathcal{H}_S . More precisely, the $S_{i_1 i_2 \dots i_N}$ are the $(N+1)$ -dimensional blocks spanned by the $|D_N^{(k)}\rangle$ ($k = 0, 1, \dots, N$) of the matrix $\mathcal{P}_S \sigma_{i_1 i_2 \dots i_N} \mathcal{P}_S^\dagger$, i.e. in terms of matrix elements

$$\langle D_N^{(k)} | S_{i_1 i_2 \dots i_N} | D_N^{(l)} \rangle = \langle D_N^{(k)} | \sigma_{i_1 i_2 \dots i_N} | D_N^{(l)} \rangle. \quad (3.15)$$

By definition, there are 4^N matrices $S_{i_1 i_2 \dots i_N}$. However, since they are invariant under permutation of indices, many of them coincide. $S_{0 \dots 0}$ is the identity matrix acting on \mathcal{H}_S . Due to the tight-frame property, one can expand any density operator of a spin- j as

$$\rho = \sum_{i_1, \dots, i_N=0}^n \frac{1}{2^N} a_{i_1 i_2 \dots i_N} S_{i_1 i_2 \dots i_N}, \quad (3.16)$$

with real and permutationally invariant coefficients

$$a_{i_1 i_2 \dots i_N} = \text{tr}(\rho S_{i_1 i_2 \dots i_N}). \quad (3.17)$$

Therefore, each density matrix ρ corresponds to a 4-dimensional tensor $\mathcal{A}_{N,4} = (a_{i_1 i_2 \dots i_N})$. Note that there are other ways than (3.17) to choose the a_{i_1, \dots, i_N} as the $S_{i_1 \dots i_N}$ form an overcomplete basis.

The representing tensor of a coherent state is particularly simple: Since any spin- j coherent state $|\alpha\rangle$ can be obtained by acting with $U = e^{-i\gamma \hat{n} \cdot \mathbf{J}}$ on $|j, j\rangle = |\frac{1}{2}, \frac{1}{2}\rangle^{\otimes N}$, a spin- j coherent state is simply a tensor product of spin-1/2 coherent states, $|\alpha\rangle_j = |\alpha\rangle_{1/2} \otimes \dots \otimes |\alpha\rangle_{1/2}$, where we have added a subscript indicating the total spin-quantum number. Since it is a symmetric state ($\mathcal{P}_S |\alpha\rangle = |\alpha\rangle$) we have

$$\langle \alpha | S_{i_1 i_2 \dots i_N} | \alpha \rangle = \langle \alpha | \mathcal{P}_S \sigma_{i_1 i_2 \dots i_N} \mathcal{P}_S^\dagger | \alpha \rangle = \langle \alpha | \otimes \dots \otimes \langle \alpha | \sigma_{i_1} \otimes \sigma_{i_2} \dots \sigma_{i_N} | \alpha \rangle \otimes \dots \otimes | \alpha \rangle \quad (3.18)$$

$$= v_{i_1} v_{i_2} \dots v_{i_N}. \quad (3.19)$$

As a consequence, $\rho = |\alpha\rangle\langle\alpha|$ has the tensor representation $a_{i_1 \dots i_N} = v_{i_1} \dots v_{i_N}$, i.e. the representing tensor \mathcal{A} of $\rho = |\alpha\rangle\langle\alpha|$ is a rank-1 tensor with $v_0 = 1$ and $\|\mathbf{v}\| = 1$.

For an arbitrary density matrix ρ , the tensor $\mathcal{A}_{N,4}$ enjoys useful properties. Firstly, the $a_{i_1 i_2 \dots i_N}$ in Eq. (3.17) are such that

$$a_{00i_3 \dots i_N} = \sum_{i=1}^3 a_{ii i_3 \dots i_N}. \quad (3.20)$$

To see this, let $|\alpha\rangle$ be a coherent state. Since its representing tensor is $a_{i_1\dots i_N} = v_{i_1} \dots v_{i_N}$, and $\mathbf{v}^2 = v_0^2 = 1$, we have

$$v_0 v_0 v_{i_3} \dots v_{i_N} = \sum_{a=1}^3 v_a v_a v_{i_3} \dots v_{i_N}, \quad (3.21)$$

which is Eq. (3.20) for coherent states. Due to the linearity of the decomposition (3.10) of ρ in terms of coherent states, Eq. (3.20) for arbitrary states follows.

Secondly, by Eqs. (3.10), (3.17) and (3.18), we have

$$\begin{aligned} a_{00\dots 0} &= \text{tr}(\rho S_{00\dots 0}) \\ &= \text{tr} \left(\int_{S^2} d\alpha P(\alpha) |\alpha\rangle \langle \alpha| S_{00\dots 0} \right) \\ &= \int_{S^2} d\alpha P(\alpha) \langle \alpha| S_{00\dots 0} |\alpha\rangle \\ &= \int_{S^2} d\alpha P(\alpha) \langle \alpha| \boldsymbol{\sigma}_{00\dots 0} |\alpha\rangle \\ &= \int_{S^2} d\alpha P(\alpha), \end{aligned} \quad (3.22)$$

so that $a_{00\dots 0} = 1$ if the state is normalized. Finally, as shown in [2], the $a_{i_1 i_2 \dots i_N}$ are unique if they are restricted to real numbers, invariant under permutation of the indices, and verifying the condition Eq. (3.20). There is therefore a mapping from the density matrices ρ of a spin- j state to 4-dimensional real symmetric normalized tensors of order $N = 2j$, $\mathcal{A}_{N,4} = (a_{i_1 i_2 \dots i_N}) \in S_{N,4}$. We call this tensor the ‘‘representing tensor’’ of the state ρ .

Hence, by Eq. (3.11), a spin- j state is classical if and only if there are positive weights $w_k > 0$ for $k = 1, \dots, r$, and vectors $\mathbf{v}^{(k)} = (1, v_1^{(k)}, v_2^{(k)}, v_3^{(k)})^\top \in \mathbb{R}^4$, satisfying

$$\left(v_1^{(k)}\right)^2 + \left(v_2^{(k)}\right)^2 + \left(v_3^{(k)}\right)^2 = 1, \quad (3.23)$$

for $k = 1, \dots, r$, such that the representing tensor $\mathcal{A} = (a_{i_1 \dots i_N}) \in S_{N,4}$ of that spin- j state satisfies

$$\mathcal{A} = \sum_{k=1}^r w_k \left(\mathbf{v}^{(k)}\right)^{\otimes N}, \quad (3.24)$$

i.e., \mathcal{A} is a regularly decomposable tensor.

Based upon the above discussions and Theorem 2.4, we have the following theorem.

Theorem 3.1 *The tensor $\mathcal{A} = (a_{i_1 \dots i_N}) \in S_{N,4}$ representing a spin- j state (with $N = 2j$) is a regular symmetric tensor. A spin- j state is classical if and only if its representing tensor is a regularly decomposable tensor.*

Thus, the physical problem of determining whether a spin- j state is classical or not is equivalent to a mathematical problem to determine whether its representing tensor is a regularly decomposable tensor or not.

4 Properties of Completely Decomposable and Regularly Decomposable Tensors

There is already substantial literature on PSD tensors and SOS tensors, including [15, 16, 17, 23, 5, 18, 19, 20, 21, 24, 22]. There are only two papers on completely decomposable tensors [23, 24]. Regularly decomposable tensors are introduced in this paper. By the discussion in the last section, we see that regularly decomposable tensors play a significant role for the classicality of spin states. Thus, in this section, we discuss properties of completely decomposable tensors and regularly decomposable tensors.

4.1 Invariance of complete decomposability and regular decomposability

Any measure of entanglement should be invariant under local unitary transformations (see e.g. [32]). Hence, also the set of fully separable states must be invariant under local unitary transformations. Correspondingly, the classicality of a spin- j state should be invariant under rotations of the coordinate system. For a physical system in three spatial dimensions, such a rotation is represented by the 3×3 orthogonal transformation matrix $R(\hat{\mathbf{n}}, \gamma)$ introduced above that acts on a vector of spatial coordinates x_1, x_2, x_3 . The corresponding transformation of a covariant tensor (i.e. a tensor that transforms as the coordinates) of dimension 4 and order m is given by its inner product with $\mathcal{R}^{\otimes m}$, where \mathcal{R} is defined by Eq. (3.13). More generally, we expect the regular decomposability of a tensor to be a property invariant under orthogonal transformations described by an $(n+1) \times (n+1)$ matrix

$$\mathcal{R} = \begin{pmatrix} 1 & \mathbf{0}^\top \\ \mathbf{0} & R \end{pmatrix},$$

where $\mathbf{0}$ is the zero vector in \mathbb{R}^n , and R is now an $n \times n$ orthogonal matrix. Then

$$R \begin{pmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ y_{n-1} \\ y_n \end{pmatrix}$$

and

$$\mathcal{R} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \cdot \\ \cdot \\ y_{n-1} \\ y_n \end{pmatrix}$$

with $x_0 = y_0$. We call such an orthogonal matrix a **normalized orthogonal matrix**. Denote $\mathcal{R} = (r_{li})$. As in [5], for any symmetric tensor $\mathcal{A} = (a_{i_1 \dots i_m}) \in S_{m, n+1}$, let $\mathcal{B} = (b_{l_1 \dots l_m}) \equiv \mathcal{R}^m \mathcal{A} \in S_{m, n}$ be defined by

$$b_{l_1 \dots l_m} = \sum_{i_1, \dots, i_m=0}^n a_{i_1 \dots i_m} r_{l_1 i_1} \dots r_{l_m i_m}$$

for $l_1, \dots, l_m = 0, \dots, n$. By [5], \mathcal{A} and \mathcal{B} have the same E-eigenvalues and Z-eigenvalues. In particular, when m is even, \mathcal{A} is PSD if and only if \mathcal{B} is PSD. By [13], when m is even, \mathcal{A} is SOS if and only if \mathcal{B} is SOS. This shows that the PSD property and the SOS property can represent physical properties, as they are invariant under orthogonal transformation.

Theorem 4.1 *Let \mathcal{R} be a normalized orthogonal matrix, $\mathcal{A}, \mathcal{B} \in S_{m,n+1}, \mathcal{B} = \mathcal{R}^m \mathcal{A}$. Then \mathcal{A} is completely decomposable if and only if \mathcal{B} is completely decomposable, and \mathcal{A} is regularly decomposable if and only if \mathcal{B} is regularly decomposable.*

Proof. Suppose that $\mathcal{A} = (a_{i_1 \dots i_m}) \in S_{m,n+1}$ is completely decomposable, $\mathcal{B} = (b_{k_1 \dots k_m}) \in S_{m,n+1}$, $\mathcal{B} = \mathcal{R}^m \mathcal{A}$, where $\mathcal{R} = (r_{li})$ is an $(n+1) \times (n+1)$ orthogonal matrix. Then there are vectors $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)} \in \mathbb{R}^{n+1}$, where $\mathbf{u}^{(k)} = (u_0^{(k)}, \dots, u_n^{(k)})^\top$ for $k = 1, \dots, r$, such that

$$\mathcal{A} = \sum_{k=1}^r \left(\mathbf{u}^{(k)} \right)^{\otimes m},$$

i.e., for $i_1, \dots, i_m = 0, \dots, n$,

$$a_{i_1 \dots i_m} = \sum_{k=1}^r u_{i_1}^{(k)} \dots u_{i_m}^{(k)}.$$

Then, for $l_1, \dots, l_m = 0, \dots, n$, we have

$$b_{l_1 \dots l_m} = \sum_{i_1, \dots, i_m=0}^n a_{i_1 \dots i_m} r_{l_1 i_1} \dots r_{l_m i_m} = \sum_{k=1}^r \sum_{i_1, \dots, i_m=0}^n u_{i_1}^{(k)} \dots u_{i_m}^{(k)} r_{l_1 i_1} \dots r_{l_m i_m} = \sum_{k=1}^r v_{l_1}^{(k)} \dots v_{l_m}^{(k)},$$

where for $k = 1, \dots, r, l = 0, \dots, n$,

$$v_l^{(k)} = \sum_{i=0}^n r_{li} u_i^{(k)}.$$

This implies that

$$\mathcal{B} = \sum_{k=1}^r \left(\mathbf{v}^{(k)} \right)^{\otimes m},$$

where $\mathbf{v}^{(k)} = (v_0^{(k)}, \dots, v_n^{(k)})^\top$ for $k = 1, \dots, r$. This implies that \mathcal{B} is completely decomposable. By [5], if $\mathcal{B} = \mathcal{R}^m \mathcal{A}$, then $\mathcal{A} = (\mathcal{R}^\top)^m \mathcal{B}$. Thus, if \mathcal{B} is completely decomposable, then \mathcal{A} is also completely decomposable.

Assume that m is even, \mathcal{A} is regularly decomposable and \mathcal{R} is a normalized orthogonal matrix. Then, we may assume that in the above discussion, vectors $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)}$ are regular. Since $\mathbf{v}^{(k)} = \mathcal{R} \mathbf{u}^{(k)}$ for $k = 1, \dots, r$, and \mathcal{R} is a normalized orthogonal matrix, we may conclude that $\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(r)}$ are also regular. This implies that \mathcal{B} is also regularly decomposable. By [5], if $\mathcal{B} = \mathcal{R}^m \mathcal{A}$, then $\mathcal{A} = (\mathcal{R}^\top)^m \mathcal{B}$. Thus, if \mathcal{B} is regularly decomposable, then \mathcal{A} is also regularly decomposable.

Now assume that m is odd, \mathcal{A} is regularly decomposable and \mathcal{R} is a normalized orthogonal matrix. Then \mathcal{B}_0 is also regularly decomposable. As \mathcal{A}_i for $i = 1, \dots, n$, are induced from the regular decomposition of \mathcal{A}_0 , we may see that \mathcal{B}_i for $i = 1, \dots, n$, are induced from the regular decomposition of \mathcal{B}_0 . This implies that \mathcal{B} is also regularly decomposable. Similarly, if \mathcal{B} is regularly decomposable, then \mathcal{A} is also regularly decomposable. \square

These show that complete decomposability and regular decomposability are invariant under normalized orthogonal transformation.

4.2 Hadamard Products

For any two tensors $\mathcal{A} = (a_{i_1 \dots i_m})$, $\mathcal{B} = (b_{i_1 \dots i_m}) \in T_{m, n+1}$, their **Hadamard product**, denoted as $\mathcal{A} \circ \mathcal{B}$, is defined by

$$\mathcal{A} \circ \mathcal{B} = (a_{i_1 \dots i_m} b_{i_1 \dots i_m}) \in T_{m, n+1}. \quad (4.25)$$

In matrix theory, the Hadamard product of two PSD symmetric matrices is also a PSD symmetric matrix. This is no longer true for tensors. In [18], an example was given that the Hadamard product of two PSD Hankel tensors may not be PSD. Hankel tensors are symmetric tensors. Thus, the Hadamard product of two PSD symmetric tensors may not be PSD. In [13], an example was given that the Hadamard product of two SOS tensors may not be an SOS tensor. However, we have the following proposition:

Proposition 4.2 *Suppose that $\mathcal{A} = (a_{i_1 \dots i_m})$, $\mathcal{B} = (b_{i_1 \dots i_m}) \in S_{m, n+1}$ are completely decomposable tensors. Then their Hadamard product $\mathcal{A} \circ \mathcal{B}$ is also a completely decomposable tensor.*

Proof. Suppose that \mathcal{A} and \mathcal{B} are completely decomposable. Then there are vectors $\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(r)}, \mathbf{v}^{(1)}, \dots, \mathbf{v}^{(p)} \in \mathfrak{R}^{n+1}$, such that

$$\mathcal{A} = \sum_{k=1}^r \left(\mathbf{u}^{(k)} \right)^{\otimes m}$$

and

$$\mathcal{B} = \sum_{l=1}^p \left(\mathbf{v}^{(l)} \right)^{\otimes m}.$$

Then is easy to see that

$$\mathcal{A} \circ \mathcal{B} = \sum_{k=1}^r \sum_{l=1}^p \left(\mathbf{u}^{(k)} \circ \mathbf{v}^{(l)} \right)^{\otimes m},$$

i.e., $\mathcal{A} \circ \mathcal{B}$ is completely decomposable. \square

This property is no longer true for regularly decomposable tensors. In this sense, completely decomposable tensors are similar to completely positive tensors studied in [20]: the Hadamard product of two completely positive tensors is still a completely positive tensor.

4.3 Duality between the PSD Tensor Cone and the Completely Decomposable Tensor Cone

Denote the set of all completely decomposable tensors in $S_{m, n+1}$ by $CD_{m, n+1}$, the set of all regularly decomposable tensors in $S_{m, n+1}$ by $RD_{m, n+1}$. Let m be even, denote the set of all PSD tensors in $S_{m, n+1}$ by $PSD_{m, n+1}$, the set of all SOS tensors in $S_{m, n+1}$ by $SOS_{m, n+1}$. Then $CD_{m, n+1}$, $RD_{m, n+1}$, $PSD_{m, n+1}$, and $SOS_{m, n+1}$ are cones.

Let C be a cone in $S_{m, n+1}$. Then its dual cone C^* is defined by

$$C^* := \{ \mathcal{A} \in S_{m, n+1} : \mathcal{A} \bullet \mathcal{B} \geq 0, \text{ for all } \mathcal{B} \in C \}.$$

The dual cone C^* is a closed convex cone. The dual cone of C^* is the closure of the convex hull of C . If C is closed and convex, then C and C^* are dual cones to each other. Let $\mathcal{A} = (a_{i_1 \dots i_m}) \in S_{m, n+1}$ and \mathfrak{R}_+^{n+1} be the nonnegative orthant of \mathfrak{R}^{n+1} . If for any $\mathbf{x} \in \mathfrak{R}_+^{n+1}$, we have $\mathcal{A} \bullet \mathbf{x}^{\otimes m} \geq 0$, then we say that \mathcal{A} is a **copositive** tensor. Copositive tensors have also applications in physics [9]. By [20], the completely positive tensor cone and copositive tensor cone are dual cones to each other.

By [33] and the definition of completely decomposable tensors, we have the following proposition.

Proposition 4.3 *Suppose that m is even. Then $PSD_{m,n+1}$ and $CD_{m,n+1}$ are dual cones to each other. Thus, both are closed convex cones.*

4.4 Closedness and Convexity of the Regularly Decomposable Tensor Cone

In the last subsection, we already knew that if m is even, then $PSD_{m,n+1}$ and $CD_{m,n+1}$ are closed convex cones. By [23], if m is odd, $CD_{m,n+1}$ is neither closed nor convex. By [13], $SOS_{m,n+1}$ is also a closed convex cone. We now discuss closedness and convexity of $RD_{m,n+1}$.

Proposition 4.4 *$RD_{m,n+1}$ is a closed convex cone.*

Proof. Suppose that $\{\mathcal{A}^{(l)} : l = 1, 2, \dots\}$ is a sequence of regularly decomposable tensors in $RD_{m,n+1}$ such that

$$\mathcal{A} = \lim_{l \rightarrow \infty} \mathcal{A}^{(l)}.$$

By Theorem 2.4, we may assume that

$$\mathcal{A}^{(l)} = \sum_{k=1}^{r_l} \alpha_{k,l} \left(\mathbf{v}^{(k,l)} \right)^{\otimes m},$$

where $\alpha_{k,l} \geq 0$, $\mathbf{v}^{(k,l)} = (1, v_1^{(k,l)}, \dots, v_n^{(k,l)})^\top$,

$$\left(v_1^{(k,l)} \right)^2 + \dots + \left(v_n^{(k,l)} \right)^2 = 1,$$

for $k = 1, \dots, r_l$, for $l = 1, 2, \dots$. By the Carathéodory theorem, we may assume that

$$r_l \leq R \equiv \binom{n+m+2}{m} + 1.$$

Thus, by taking a subsequence if necessary, without loss of generality, there is a $r \leq R$ such that $r_l = r$ for $l = 1, 2, \dots$. Then, we may conclude that there are $\alpha_k \geq 0$, $\mathbf{v}^{(k)} = (1, v_1^{(k)}, \dots, v_n^{(k)})^\top$,

$$\left(v_1^{(k)} \right)^2 + \dots + \left(v_n^{(k)} \right)^2 = 1,$$

for $k = 1, \dots, r$. Thus, by Theorem 2.4, \mathcal{A} is a regularly decomposable tensor. This shows that $RD_{m,n+1}$ is a closed cone. Similarly, we prove that $RD_{m,n+1}$ is a convex cone. \square

5 Concluding Remarks

In this paper, we have introduced the concept of regularly decomposable tensors. We have shown that a spin state is classical if and only if its representing tensor is a regularly decomposable tensor. Thus, the problem for determining whether a spin state is classical or not is mathematically equivalent to the problem of determining whether a given regular symmetric tensor is a regularly decomposable tensor or not.

How can we construct an algorithm for determining a given regular symmetric tensor is a regularly decomposable tensor or not? We see that the properties of completely decomposable tensors and regularly decomposable tensors in some extent are similar to those of completely positive tensors [34, 20]. Recently, an algorithm for determining whether a given symmetric nonnegative tensor is completely positive or not was proposed [35]. Perhaps we may learn from that algorithm how to construct an algorithm determining whether a given regular symmetric tensor is regularly decomposable or not.

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A.6. Entanglement and the truncated moment problem

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Entanglement and the truncated moment problem

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We map the quantum entanglement problem onto the mathematically well-studied truncated moment problem. This yields a necessary and sufficient condition for separability that can be checked by a hierarchy of semi-definite programs. The algorithm always gives a certificate of entanglement if the state is entangled. If the state is separable, typically a certificate of separability is obtained in a finite number of steps and an explicit decomposition into separable pure states can be extracted.

I. INTRODUCTION

The renewed interest that entanglement theory attracted in the last decades has led to a tremendous amount of new results (see the recent reviews [1–4] and references therein). Still, characterization and detection of multipartite entanglement is largely an open question. For quantum states describing a collection of qubits, the size of Hilbert space, exponential in the number of qubits, makes the problem daunting. A simpler but still challenging problem is to restrict the question of characterizing entanglement to a smaller set of quantum states, such as for instance symmetric states, which are pure states invariant under permutations of constituents, or mixtures thereof. Symmetric states lie in a Hilbert space of size linear in the number of qubits, which makes the investigation more tractable. Once the symmetric case is understood, it can shed light onto the general case. This is the strategy we will follow here, first considering the symmetric case, which is easier to handle and to present from a pedagogical point of view, then extending our results to the fully general non-symmetric case.

Various results on entanglement for symmetric states have been obtained in the literature [5–9]. For instance, criteria for certifying separability in symmetric mixed states of N qubits were found in [10]. Separable symmetric N -qubit pure states are always fully separable [11]. They are easily characterized, as there is a one-to-one correspondence between these states and points on the Bloch sphere via the Majorana representation [12]. As will be detailed in the paper, a symmetric state is separable (that is, it can be written as a convex combination of separable pure states) if and only if it can be associated with a probability distribution on the sphere; this measure then gives the positive weights associated with each separable pure state. A convenient representation to describe symmetric states in terms of symmetric tensors was proposed in [13], generalizing the Bloch sphere picture of spins-1/2. In terms of this tensor representation, decomposing a state into a convex combination of separable pure states amounts to finding a probability distribution whose lowest-order moments are fixed by the tensor entries. In fact, as we will see, the generic problem of finding whether an arbitrary (not necessarily symmetric) multipartite state can be decomposed into

product states can be cast into the problem of finding a probability distribution whose lowest-order moments are fixed.

The problem of finding a probability distribution from the knowledge of its moments has been extensively studied in the literature. When only a finite number of moments is known, the problem is to find a probability distribution compatible with these moments. In the case of multivariate distributions, it corresponds to the so-called *truncated moment problem*: given a truncated moment sequence (tms), that is, fixing all moments up to a certain order, is there a probability distribution (or, in mathematical terms, a nonnegative measure) whose moments coincide with those of the tms? When it exists, such a measure is called a representing measure of the tms. Of practical relevance is the closely related K -tms problem, where the measure reproducing the fixed moments is constrained to be supported on some compact K .

The non-truncated K -moment problem, where all moments are given, was solved in [14] in the case where the compact K is semi-algebraic (i.e. defined by polynomial inequalities). For the K -tms problem (and for K semi-algebraic), Curto and Fialkow [15] obtained a necessary and sufficient condition for a tms to admit a representing measure (see Theorem 1 below). In [16], a semidefinite algorithm was introduced, allowing one to find a representing measure (if it exists), and later generalized to situations where only a subset of moments up to a certain order are known [17]. This algorithm was also used in [18] to test positivity of linear maps and separability of matrices in relation with the entanglement problem. More detail on the history of the tms problem can be found in the review [19].

The goal of the present paper is to show how the separability problem for an arbitrary quantum state can be mapped to the K -tms problem, and to use results from the tms literature to elucidate some aspects of entanglement detection and characterization of separability. From an analytical point of view, the mapping allows us to make use of theorems providing necessary and sufficient separability conditions. Numerically, semi-definite programming yields an algorithm to obtain an explicit decomposition of separable states.

The idea of using semi-definite programming to test for entanglement was already proposed in [20–22] by Doherty, Parrilo, and Spedalieri, and independently in [23].

In [21] an algorithm was provided which detects entanglement, but this algorithm never stops if the state is separable. Conversely, the algorithm proposed in [24] detects separable states but does not certify entanglement. The algorithms in [20–22] use the concept of “extensions”, i.e. states in a larger Hilbert space are considered, such that their partial trace gives back the original state. By going to larger and larger extensions, a hierarchy of semi-definite programs (SDPs) arises whose infeasibility at any stage signals that the original state ρ_{AB} is entangled. The authors of [20–22] add the request that the extensions have positive partial transpose (i.e. are “PPT”) as a necessary criterion for separability. This additional condition can be implemented at little extra cost in the SDP. Furthermore, they search in the space of “ N Bose-symmetric extensions”, where the extended state ρ_{AB^N} (besides being positive semi-definite and reproducing $\rho_{AB} = \text{tr}_{B^{N-1}}[\rho_{AB^N}]$) is invariant under projection onto the symmetric subspace of B^N . These algorithms were further improved in [25–28].

The algorithm we propose here gives a unifying mathematical framework that also uses semi-definite programming and extensions, but in a somewhat more abstract way, based on a matrix of moments and a theorem in the theory of moment sequences. It provides an elegant solution of the entanglement problem, and in particular provides a certificate of separability, together with an explicit decomposition into product states if the state is separable. Moreover, it applies to arbitrary quantum state with arbitrary number of constituents and arbitrary symmetries between the subparts and easily accomodates missing data, i.e. incompletely specified states.

After setting up the notations, we define the K -tms problem (Section II), explain the procedures and algorithms allowing to solve it (Section III) and then show explicit numerical results (Section IV). In Section V we show that, conversely, some solutions of the entanglement problems may shed light on a particular tms problem. A discussion of the advantages and novelties of our treatment compared to previous algorithms is provided in the conclusions.

II. ENTANGLEMENT AND THE TRUNCATED MOMENT PROBLEM

To familiarize the reader with the notations in this paper, we will first consider the case of symmetric states of qubits, since in this case the equations are more compact. After that we will explain the general case in the following subsection.

A. Symmetric qubit case

Multi-qubit pure states which are invariant under any permutation of the qubits are called symmetric pure states. Symmetric states are mixtures of symmetric pure

states. Such states are formally equivalent to spin states with spin quantum number $N/2$, where N is the number of qubits. This connection can be made explicit with the Dicke states defined by

$$|D_N^{(k)}\rangle = \mathcal{N} \sum_{\pi} | \underbrace{0 \dots 0}_k \underbrace{1 \dots 1}_{N-k} \rangle, \quad (1)$$

where \mathcal{N} is a normalization constant and the sum runs over all permutations of the qubits. These states with $k \in \{0, \dots, N\}$ form a basis of the symmetric subspace of the Hilbert space \mathbb{C}^{2^N} of N qubits. We now introduce a convenient way of representing symmetric states as tensors. For a state ρ , let

$$X_{\mu_1 \mu_2 \dots \mu_N} = \text{tr} \{ \rho P_s^\dagger \sigma_{\mu_1} \otimes \dots \otimes \sigma_{\mu_N} P_s \}, \quad (2)$$

with σ_0 the 2×2 identity matrix, $\sigma_1, \sigma_2, \sigma_3$ the three Pauli matrices, and P_s the projector onto the symmetric subspace spanned by Dicke states (1). Then ρ can be expanded [13] as

$$\rho = \frac{1}{2^N} X_{\mu_1 \mu_2 \dots \mu_N} P_s^\dagger \sigma_{\mu_1} \otimes \dots \otimes \sigma_{\mu_N} P_s \quad (3)$$

(with summation over repeated indices). The tensor $X_{\mu_1 \mu_2 \dots \mu_N}$ is real and invariant under permutation of indices, and verifies

$$X_{0 \dots 0} = \text{tr} \rho = 1. \quad (4)$$

In this representation, the tensor associated with a pure separable symmetric state $|\psi_{sep}\rangle$ of N qubits takes the particularly simple form

$$X_{\mu_1 \mu_2 \dots \mu_N} = n_{\mu_1} \dots n_{\mu_N} \quad (5)$$

with $n_0 = 1$ and $\mathbf{n} = (n_1, n_2, n_3)$ the Bloch vector of the individual qubit, $n_1^2 + n_2^2 + n_3^2 = 1$. Note that since the state is invariant under the exchange of qubits, a pure state can only be the tensor product of identical qubits (with same Bloch vector \mathbf{n}), and a separable pure symmetric state has to be fully separable [29]. As a consequence, a symmetric state is separable if and only if its tensor representation can be written as

$$X_{\mu_1 \mu_2 \dots \mu_N} = \sum_j w_j n_{\mu_1}^{(j)} \dots n_{\mu_N}^{(j)}, \quad (6)$$

with $w_j \geq 0$, $n_0^{(j)} = 1$ and each Bloch vector $\mathbf{n}^{(j)}$ normalized to 1. This can be equivalently written in an integral form as

$$X_{\mu_1 \mu_2 \dots \mu_N} = \int_K x_{\mu_1} x_{\mu_2} \dots x_{\mu_N} d\mu(\mathbf{x}), \quad (7)$$

with $K = \{\mathbf{x} \in \mathbb{R}^3 : x_1^2 + x_2^2 + x_3^2 = 1\}$ the unit sphere, $x_0 = 1$, and $d\mu$ a positive measure on K . Indeed, if (6) holds then the tensor can be written as in (7) with

$$d\mu(\mathbf{x}) = \sum_j w_j \delta(\mathbf{x} - \mathbf{n}^{(j)}). \quad (8)$$

Conversely, since the system is finite-dimensional, Carathéodory's theorem implies that the integral in (7) can always be reduced to a finite sum as in (6), so that the positive measure can always be expressed as a sum of delta functions. Expressing Eq. (7) in words, a symmetric state is separable if and only if there exist a positive measure $d\mu$ such that all entries of the tensor $X_{\mu_1\mu_2\dots\mu_N}$ (for all μ_j , $1 \leq j \leq N$ and $0 \leq \mu_i \leq 3$) are given by moments of that measure.

In order to prepare for the generalization to arbitrary states in the next subsection, let us introduce a more compact notation for Eq. (7). For any N -tuple (μ_1, \dots, μ_N) we define a triplet $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ of integers such that

$$x_{\mu_1} x_{\mu_2} \cdots x_{\mu_N} = x^\alpha, \quad (9)$$

where we use the notation $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3}$. So e.g. for $\alpha = (1, 3, 0)$ we have $x^\alpha = x_1 x_2^3$. The degree of the monomial x^α is denoted $|\alpha| \equiv \sum_i \alpha_i$. We also denote the $X_{\mu_1\mu_2\dots\mu_N}$ by y_α , where α corresponds to $(\mu_1\mu_2\dots\mu_N)$ via Eq. (9), so that e.g. for $N = 6$, $y_{(2,1,0)} = X_{000112}$. With this notation we can rewrite (7) as

$$y_\alpha = \int_K x^\alpha d\mu(\mathbf{x}). \quad (10)$$

To test if a symmetric state is separable, a necessary and sufficient condition is therefore that a positive measure $d\mu$ exists that fulfills (10) for all $|\alpha| \leq N$. Problems of this type are known as *truncated K -moment sequence problems* (or *K -tms problems*), and they can be solved by a semi-definite relaxation procedure. Before we describe this method in Section III we generalize the description to arbitrary states of finite-dimensional systems.

B. General case

Consider a multipartite quantum state ρ acting on the tensor product $\mathcal{H} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \cdots \otimes \mathcal{H}^{(d)}$ of Hilbert spaces $\mathcal{H}^{(i)}$. For each i , let $S_{\mu_i}^{(i)}$, $0 \leq \mu_i \leq t_i$ be a set of $t_i + 1$ Hermitian matrices forming an orthogonal basis (with respect to the scalar product $\text{tr} A^\dagger B$) of the set of bounded linear operators on $\mathcal{H}^{(i)}$, with the choice that $S_0^{(i)}$ is the identity matrix. An orthogonal basis of \mathcal{H} is then given by matrices

$$S_{\mu_1\mu_2\dots\mu_d} = S_{\mu_1}^{(1)} \otimes S_{\mu_2}^{(2)} \otimes \cdots \otimes S_{\mu_d}^{(d)} \quad (11)$$

and any state can be written as

$$\rho = \mathcal{N} X_{\mu_1\mu_2\dots\mu_d} S_{\mu_1\mu_2\dots\mu_d} \quad (12)$$

where summation over repeated indices is understood, and the normalization constant $\mathcal{N} = \prod_{i=1}^d \mathcal{N}_i$, with $\mathcal{N}_i = 1/\sqrt{t_i + 1}$, is chosen so that $X_{0\dots 0} = 1$. A quantum state ρ_{sep} is said to be separable (over that particular factorization of \mathcal{H}) if it can be written as

$$\rho_{sep} = \sum_j w_j \rho_j^{(1)} \otimes \rho_j^{(2)} \otimes \cdots \otimes \rho_j^{(d)} \quad (13)$$

with $w_j \geq 0$, and $\rho_j^{(i)}$ density matrices acting on $\mathcal{H}^{(i)}$ [30]. Any $\rho^{(i)}$ acting on $\mathcal{H}^{(i)}$ can be expanded as $\rho^{(i)} = \mathcal{N}_i \sum_{\mu_i} y_{\mu_i}^{(i)} S_{\mu_i}^{(i)}$, with $y^{(i)}$ a real $(t_i + 1)$ -dimensional vector. The condition $\text{tr} \rho^{(i)} = 1$, together with the choice that $S_0^{(i)}$ is the identity matrix and the normalization, implies that $y_0^{(i)} = 1$.

Rewriting condition (13) in terms of average values, we get that a state is fully separable if and only if all averaged basis operators can be expressed as

$$\langle S_{\mu_1\mu_2\dots\mu_d} \rangle_\rho = \sum_j w_j \langle S_{\mu_1}^{(1)} \rangle_{\rho_j^{(1)}} \langle S_{\mu_2}^{(2)} \rangle_{\rho_j^{(2)}} \cdots \langle S_{\mu_d}^{(d)} \rangle_{\rho_j^{(d)}} \quad (14)$$

with $w_j \geq 0$, i.e. the expectation values of all $S_{\mu_1\mu_2\dots\mu_d}$ are convex combinations of the product of local expectation values. This condition can be reexpressed in terms of the coefficients $X_{\mu_1\mu_2\dots\mu_d}$ of ρ_{sep} in the expansion (12) and the coefficients $y_{a_i}^{(i;j)}$, $1 \leq a_i \leq t_i$, in the expansion $\rho_j^{(i)} = \mathcal{N}_i \sum_{\mu_i} y_{\mu_i}^{(i;j)} S_{\mu_i}^{(i)}$, with $y_0^{(i;j)} = 1$. Separability is then equivalent to the existence of $w_j \geq 0$ and real numbers $y_{a_i}^{(i;j)}$, $1 \leq a_i \leq t_i$, such that for all μ_i with $0 \leq \mu_i \leq t_i$ one has

$$X_{\mu_1\mu_2\dots\mu_d} = \sum_j w_j y_{\mu_1}^{(1;j)} y_{\mu_2}^{(2;j)} \cdots y_{\mu_d}^{(d;j)} \quad (15)$$

and $\sum_{\mu_i} y_{\mu_i}^{(i;j)} S_{\mu_i}^{(i)} \geq 0$ for all i and j . This latter condition comes from the fact that each $\rho_j^{(i)} = \mathcal{N}_i \sum_{\mu_i} y_{\mu_i}^{(i;j)} S_{\mu_i}^{(i)}$ appearing in (13) is a density matrix, and thus has to be positive. Since matrices are Hermitian and thus have all their eigenvalues real, one can use Descartes sign rule to express this positivity condition as inequalities on the coefficients of the characteristic polynomial of $\rho_j^{(i)}$. Each of these coefficient is a linear combination of traces of powers of $\rho_j^{(i)}$, and therefore a polynomial in the variables $y_{\mu_i}^{(i;j)}$. Thus, each vector $\mathbf{y}^{(i;j)} = (y_1^{(i;j)}, \dots, y_{t_i}^{(i;j)})$ is restricted to a certain compact subset $K^{(i)} \subset \mathbb{R}^{t_i}$ defined by some polynomial inequalities, e.g. for a qubit the polynomial is a quadratic equation of the Bloch vector, restricting its maximal length to one. Defining the compact $K = K^{(1)} \times K^{(2)} \times \cdots \times K^{(d)} \subset \mathbb{R}^n$, $n = \sum_i t_i$, and the vector $\mathbf{y}^{(j)} = (\mathbf{y}^{(1;j)}, \mathbf{y}^{(2;j)}, \dots, \mathbf{y}^{(d;j)}) \in \mathbb{R}^n$, the positivity condition on the partial density matrices amounts to impose that $\mathbf{y}^{(j)} \in K$ with K a compact defined by polynomial inequalities. Equation (15) can then be rewritten, for $0 \leq \mu_i \leq t_i$, as

$$X_{\mu_1\mu_2\dots\mu_d} = \int_K x_{\mu_1}^{(1)} x_{\mu_2}^{(2)} \cdots x_{\mu_d}^{(d)} d\mu(\mathbf{x}) \quad (16)$$

with $x_0^{(i)} = 1$, $\mathbf{x} = (\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(d)}) \in \mathbb{R}^n$, $\mathbf{x}^{(i)} = (x_a^{(i)})_{1 \leq a \leq t_i} \in \mathbb{R}^{t_i}$, and $d\mu$ the measure over \mathbb{R}^n defined

by

$$d\mu(\mathbf{x}) = \sum_j w_j \delta(\mathbf{x} - \mathbf{y}^{(j)}). \quad (17)$$

Equation (16) is the generalization of the symmetric case Eq. (7), the difference being that each Hilbert space $\mathcal{H}^{(i)}$ has its own set of variables $(x_a^{(i)})_{1 \leq a \leq t_i}$. As in the symmetric case, the existence of an arbitrary measure $d\mu(\mathbf{x})$ such that (16) holds is equivalent to the existence of a 'discrete' measure of the form (17), since one can apply Carathéodory's theorem to our finite dimensional Hilbert spaces. The separability problem, for a state given by (12), is thus equivalent to the question whether a positive measure $d\mu$ with support K exists whose moments coincide with the coordinates $X_{\mu_1 \mu_2 \dots \mu_d}$ of the state.

We now rewrite Eq. (16) in a more compact form. Let us relabel the entries of \mathbf{x} as $\mathbf{x} = (x_1, x_2, \dots, x_n)$, and introduce the notation $x^\alpha \equiv \prod_{i=1}^n x_i^{\alpha_i}$, where $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)$ is a vector of integers. For instance for two qubits we have $\mathbf{x} = (x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, x_1^{(2)}, x_2^{(2)}, x_3^{(2)}) = (x_1, x_2, \dots, x_6)$. For any given tuple (μ_1, \dots, μ_d) , there exists an index α such that

$$x_{\mu_1}^{(1)} x_{\mu_2}^{(2)} \dots x_{\mu_d}^{(d)} = x^\alpha. \quad (18)$$

Thus, α_1 counts the number of $x_1^{(1)}$ in the monomial $x_{\mu_1}^{(1)} x_{\mu_2}^{(2)} \dots x_{\mu_d}^{(d)}$, α_2 counts the number of $x_2^{(1)}$, and so on until α_n , which counts the number of $x_{t_d}^{(d)}$. For instance for a bipartite state of $d = 2$ qubits, $(\mu_1, \mu_2) = (2, 3)$ corresponds to $\alpha = (0, 1, 0, 0, 0, 1)$ or to the monomial $x_2^{(1)} x_3^{(2)}$, while $(\mu_1, \mu_2) = (1, 0)$ corresponds to $\alpha = (1, 0, 0, 0, 0, 0)$ or to the monomial $x_1^{(1)}$. As each monomial $x_{\mu_1}^{(1)} x_{\mu_2}^{(2)} \dots x_{\mu_d}^{(d)}$ contains at most one variable of each type $x^{(i)}$, the vector α is such that each tuple $(\alpha_1, \dots, \alpha_{t_1}), (\alpha_{t_1+1}, \dots, \alpha_{t_1+t_2}), \dots$, contains at most one 1. For instance for qubits, where $t_i = 3$, each triplet $(\alpha_{3i+1}, \alpha_{3i+2}, \alpha_{3i+3})$ must therefore contain at most one 1.

If we denote $X_{\mu_1 \mu_2 \dots \mu_d}$ by y_α , where α is the index corresponding to the tuple (μ_1, \dots, μ_d) via (18), then Eq. (16) can be simply rewritten as

$$y_\alpha = \int_K x^\alpha d\mu(\mathbf{x}). \quad (19)$$

Hence, a state is separable if and only if all its coordinates y_α can be written as in Eq. (19), with $d\mu$ a positive measure.

C. Examples and special cases

The general setting of the previous Subsection allows one to test separability for a given fixed partition. For example, in order to check full separability for a three-qubit state ρ one has to consider $d = 3$ sets of variables

$x_{a_i}^{(i)}$, each set being associated with a qubit (thus with $1 \leq a_i \leq 3$), and K is the product of three Bloch spheres. One then relabels the coordinates $X_{\mu_1 \mu_2 \mu_3}$ of ρ as y_α and the variables as (x_1, \dots, x_n) with $n = 9$, in order to get Eq. (19). Among all 9-tuples $\alpha = (\alpha_1, \dots, \alpha_n)$, only the 64 values which correspond to some triplet (μ_1, μ_2, μ_3) for $0 \leq \mu_i \leq 3$ via (18) have to be considered. The state ρ is separable if and only if there exists a measure $d\mu$ such that Eq. (19) is fulfilled for all these α .

However if one is only interested in the question of entanglement of the first two qubits with respect to the third one, one would have to take the first two qubits as a 4-level system. There would then be two sets of variables in Eq. (16), the first one with $t_1 = 15$ variables (characterizing the density matrix of a 4-level system), and the second with $t_2 = 3$ variables (characterizing a mixed qubit state). Thus one has $d = 2$ and $n = 18$ variables. Finding whether or not (19) can be solved answers the question whether or not the third qubit is entangled with the first two, while ignoring any entanglement between the first two qubits.

It is instructive to see how the symmetric case of Subsection II A can be recovered from the general case. As we saw in Subsection II A, the problem of finding whether a symmetric N -qubit state is fully separable can be cast into the form (10), with K the 2-sphere and α running over triplets of integers with $|\alpha| \leq N$. Applying the general case to the N -qubit case implies $d = N$ parties, and the Hilbert space \mathcal{H} is decomposed as $\mathcal{H} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \dots \otimes \mathcal{H}^{(N)}$. Each Hilbert space $\mathcal{H}^{(i)}$ has its own set of variables $x_{a_i}^{(i)}$, $1 \leq a_i \leq 3$, appearing in the right-hand side of Eq. (16). The basis $S_\mu^{(i)}$ in the decomposition $\rho^{(i)} = \frac{1}{2} \sum_\mu y_\mu^{(i)} S_\mu^{(i)}$ is the Pauli basis, the vectors $(y_a^{(i)})_{1 \leq a \leq 3}$ are the Bloch vectors and the compact $K^{(i)}$ such that $\sum_\mu y_\mu^{(i)} S_\mu^{(i)}$ is positive is the Bloch ball. Symmetry then implies that the variables corresponding to each Hilbert space are not independent but equal, so that one has to require $x_\mu^{(i)} = x_\mu$ for all i and μ , and replace the compact $K^{(1)} \times K^{(2)} \times \dots \times K^{(d)}$ by $K = K^{(1)}$, a single Bloch sphere. To account for the fact that the different sets of variables should no longer be distinguished, the n -tuple α in (19) should be replaced by the triplet $(\sum_i \alpha_{3i+1}, \sum_i \alpha_{3i+2}, \sum_i \alpha_{3i+3})$ giving the multiplicities of x_1, x_2, x_3 . The entries of the triplet can now take values larger than one. Since Eq. (19) and Eq. (10) coincide, the symmetric and the general case are in essence the same problem; the difference between them lies only in the definition of the compact K supporting the measure, and also in the set of tuples α considered.

The general formalism (19) allows us in fact to play with any kind of constraint, just by adjusting the sets of variables and α vectors accordingly. The symmetric case explained above is just one example, but this method is general. For instance if one wants to impose a symmetry between two of the subsystems one just has to equate the sets of independent variables. This adjustment can

be easily generalized to test for entanglement for any type of partition. The algorithms for the truncated moment problem that we will present in Section III provide a solution to all these cases.

D. Partial knowledge of a state

An interesting question in practical application is whether or not a partial set of measurement results is compatible with a separable state. If for example a state tomography is not carried to its end, or if only local measurements are available, can one in some instances infer that the state was entangled? Another interesting question is whether the partial traces of a state can be used to show entanglement of the global state even if all the reduced states are separable [31].

Such problems of partial knowledge can be formulated in the form of Eq. (19) very simply. The only change is the range of tuples over which α varies: since the unknown measurements correspond to unknown y_α , these values of α should not be taken into account as constraints on $d\mu$. If for example only the results of local measurements are known, only averages of the form $\langle S_0^{(1)} \otimes S_0^{(2)} \otimes \dots \otimes S_\mu^{(i)} \dots \otimes S_0^{(d)} \rangle$ are known (recall that $S_0^{(i)}$ is the identity matrix). Therefore one only knows the values of y_α such that the $\alpha = (\alpha_1, \dots, \alpha_n)$ have only one non-zero entry. This problem can then be solved in the same way as the general one, just by putting no constraint on the unknown moments.

III. TMS PROBLEMS: DEFINITIONS AND SOLUTIONS

Identifying the entanglement problem with the K -tms problem allows us to use analytical results and numerical methods from the tms literature to get insight in entanglement theory. We now introduce the mathematical formalism used to describe and solve the tms problem.

A. Truncated moment problems

A truncated moment sequence (tms) of degree d is a finite set of numbers $y = (y_\alpha)_{|\alpha| \leq d}$ indexed by n -tuples $\alpha = (\alpha_1, \dots, \alpha_n)$ of integers $\alpha_i \geq 0$ such that $|\alpha| = \sum_i \alpha_i \leq d$ [17]. The truncated K -moment problem consists in finding conditions under which there exists a (positive) measure $d\mu$ such that each moment y_α with $|\alpha| \leq d$ can be represented as an integral of the form

$$y_\alpha = \int_K x^\alpha d\mu(\mathbf{x}) \quad (20)$$

with $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$, $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_n^{\alpha_n}$, and $d\mu$ a measure supported on a semi-algebraic set

$$K = \{\mathbf{x} \in \mathbb{R}^n | g_1(\mathbf{x}) \geq 0, \dots, g_m(\mathbf{x}) \geq 0\} \quad (21)$$

with $g_i(\mathbf{x})$ multivariate polynomials in the variables x_1, \dots, x_n . If such a measure exists it can be written as the sum of delta functions

$$d\mu(\mathbf{x}) = \sum_{j=1}^r w_j \delta(\mathbf{x} - \mathbf{y}^{(j)}) \quad (22)$$

with some finite r , $w_j > 0$ and $\mathbf{y}^{(j)} \in K$. Such a measure is then called a *finitely atomic representing measure*. Equation (20) is nothing but Eq. (10), where K is the Bloch sphere, $d = N$, and $n = 3$. Therefore the entanglement problem for symmetric states is a special case of K -tms problem.

The \mathcal{AK} -tms problem [17] is a generalization of the K -tms problem in which moments y_α are known only for a finite subset $\mathcal{A} \subset \mathbb{N}^n$ of indices of degree $|\alpha| \leq d$. The only difference with the K -tms problem is that Eq. (20) now has to be fulfilled only for $\alpha \in \mathcal{A}$. This is exactly the situation found in the general case of Subsection II B. Indeed, in that case, we showed that K is defined by polynomial inequalities, so that it is a semi-algebraic compact set. Moreover, only indices α associated with some tuple (μ_1, \dots, μ_d) for $0 \leq \mu_i \leq t_i$ do correspond to a certain moment y_α , so that a restriction on indices α is required. This is also the situation encountered in Subsection II D, where the state is only known partially. All these cases therefore correspond to the \mathcal{AK} -tms problem, and can in fact be solved in the same way as the K -tms problem, only with fewer constraints (since less moments are fixed).

In all what follows, to ease notations, we will only treat the original K -tms problem where all moments y_α with $|\alpha| \leq d$ are known. However, we must stress that the \mathcal{AK} -tms problem is treated in exactly the same way, just by considering $\alpha \in \mathcal{A}$ rather than $|\alpha| \leq d$ in all equations involving that restriction.

B. Moment matrices

Let us now present the mathematical setting for the K -tms problem defined by Eq. (20). Let $y = (y_\alpha)_{|\alpha| \leq d}$ be a tms of degree d , with $\alpha = (\alpha_1, \dots, \alpha_n)$ being n -tuples of integers. The integrand in the right-hand side of Eq. (20) is a monomial in n variables (x_1, \dots, x_n) of degree less than d . Any polynomial of degree less than d can be written as a vector in the basis of monomials ordered in degree-lexicographic order (that is, monomials are sorted by order and within each order in a lexicographic order). For instance for $n = 3$ and $d = 2$ the monomial basis is $\{1, x_1, x_2, x_3, x_1^2, x_1 x_2, x_1 x_3, x_2^2, x_2 x_3, x_3^2\}$, and a polynomial such as e.g. $p(\mathbf{x}) = 7x_3 - 3x_2^2 + 2$ would be written as the vector $(2, 0, 0, 7, 0, 0, 0, -3, 0, 0)$. The components of the vector representing $p(\mathbf{x})$ are coefficients p_α such that $p(\mathbf{x}) = \sum_\alpha p_\alpha x^\alpha$.

For any integer $k \leq d/2$, let $M_k(y)$ be the matrix defined by

$$M_k(y)_{\alpha\beta} = y_{\alpha+\beta}, \quad |\alpha|, |\beta| \leq k. \quad (23)$$

It is called the *moment matrix* of order k associated with the tms y . A necessary condition for a tms to admit a representing measure as in (20) is that the moment matrix of any order is positive-semidefinite. Indeed, if (20) holds, then for any vector $p = (p_\alpha)_{|\alpha| \leq k}$ representing a polynomial $p(\mathbf{x})$ of degree k or less we have

$$p^T M_k(y) p = \sum_{|\alpha|, |\beta| \leq k} p_\alpha y_{\alpha+\beta} p_\beta = \sum_{|\alpha|, |\beta| \leq k} p_\alpha p_\beta \int_K x^{\alpha+\beta} d\mu(\mathbf{x}) = \int_K p(\mathbf{x})^2 d\mu(\mathbf{x}) \geq 0, \quad (24)$$

so that $M_k(y)$ is a positive-semidefinite matrix [15, 16].

Other necessary conditions can be obtained from the polynomial constraints $g_i(\mathbf{x}) \geq 0$ which define the set K in (21). For any polynomial g of degree $\deg(g) \geq 1$, one can define a 'shifted tms' of degree $d - \deg(g)$ as

$$(g \star y)_\alpha = \sum_{|\gamma| \leq \deg(g)} g_\gamma y_{\alpha+\gamma}, \quad |\alpha| \leq d - \deg(g). \quad (25)$$

Let $d_g = \lceil \deg(g)/2 \rceil$ (we denote by $\lceil x \rceil$ the smallest integer larger than x and by $\lfloor x \rfloor$ the largest integer smaller than x). Applying definition (23), one can define the $(k - d_g)$ th moment matrix of $g \star y$, for any integer k such that $0 \leq k - d_g \leq \lfloor d - \deg(g) \rfloor / 2$, by $M_{k-d_g}(g \star y)_{\alpha\beta} = (g \star y)_{\alpha+\beta}$. This matrix is called the k th-order *localizing matrix* of g [16]. In explicit form, it reads

$$M_{k-d_g}(g \star y)_{\alpha\beta} = \sum_{|\gamma| \leq \deg(g)} g_\gamma y_{\alpha+\beta+\gamma}, \quad |\alpha|, |\beta| \leq k - d_g. \quad (26)$$

Using the fact that $\lfloor (d - \deg(g))/2 \rfloor = \lfloor d/2 \rfloor - d_g$, we have that the k th-order localizing matrix is defined for any integer k such that $d_g \leq k \leq d/2$ (the definition of d_g has been precisely chosen in such a way that the upper bound $k \leq d/2$ is the same as that for the k th-order moment matrix). If a tms admits a representing measure then any k th order localizing matrix is necessarily positive-semidefinite: indeed for any vector $p = (p_\alpha)_{|\alpha| \leq k - d_g}$ representing a polynomial $p(\mathbf{x})$ with degree $k - d_g$ or less we have

$$p^T M_{k-d_g}(g \star y) p = \sum_{|\alpha|, |\beta| \leq k - d_g} p_\alpha p_\beta \sum_{|\gamma| \leq \deg(g)} g_\gamma y_{\alpha+\beta+\gamma} = \int_K g(\mathbf{x}) p(\mathbf{x})^2 d\mu(\mathbf{x}) \geq 0, \quad (27)$$

which is positive because g is positive on K by the definition (21). Another way of seeing that is to observe that if y admits a positive representing measure then so does the shifted tms $g \star y$.

As moment matrices of order k' are submatrices of matrices of order k if $k' \leq k$ it suffices to consider the largest possible value for k to get the strongest necessary conditions. For a tms y of order d , the above analysis leads to the necessary condition $M_{\lfloor d/2 \rfloor}(y) \geq 0$. If the compact K is defined as in (21) by polynomial inequalities, the localizing matrices for each polynomial g_i , $1 \leq i \leq m$, have to be positive, namely $M_{\lfloor d/2 \rfloor - d_{g_i}}(g_i \star y) \geq 0$, $d_{g_i} = \lceil \deg(g_i)/2 \rceil$.

C. A necessary and sufficient condition

The above conditions are only necessary conditions. A sufficient condition was obtained in [15] for even-order tms. We formulate it following Theorem 1.1 of [16]. Namely, if a tms z of even order $2k$ is such that its k th order moment matrix and all k th order localizing matrices are positive, and if additionally

$$\text{rank} M_k(z) = \text{rank} M_{k-d_0}(z) \quad (28)$$

with $d_0 = \max_{1 \leq i \leq m} \{1, \lceil \deg(g_i)/2 \rceil\}$, then the tms z admits a representing measure composed of $r = \text{rank} M_k(z)$ delta functions. Note that the rank condition already appeared in [25] under the name rank-loop, using a result from [32].

As the above condition is only sufficient, a tms y admitting a representing measure does not necessarily fulfill (28). However, one can search for an extension z of y which fulfills it. An extension of a tms y of degree d is defined as any tms z of degree $2k$ with $2k > d$, such that $z_\alpha = y_\alpha$ for all $|\alpha| \leq d$. A extension z is called flat if it satisfies Eq. (28). If z verifies the sufficient conditions above, then it has a representing measure, and so does y as a restriction of z . This allows us to formulate the following necessary and sufficient condition for the existence of a representing measure.

Theorem 1 ([15] (see also Theorem 1.2 of [16])). *A tms $(y_\alpha)_{|\alpha| \leq d}$ admits a representing measure supported by K if and only if there exists a flat extension $(z_\beta)_{|\beta| \leq 2k}$ with $2k > d$ such that $M_k(z) \geq 0$, and $M_{k-d_{g_i}}(g_i \star z) \geq 0$ for $i = 1, \dots, m$.*

This theorem can be implemented as a semi-definite program, as shown in Section III D. It has been extended to an arbitrary \mathcal{AK} -tms in proposition 3.3 in [17]. With the identifications made in Sec. II between the entanglement and the tms problem, these results can be reformulated as a necessary and sufficient condition for separability of an arbitrary quantum state:

Theorem 2. *A state ρ is separable if and only if its coordinates $X_{\mu_1 \mu_2 \dots \mu_d}$ defined in (12) correspond to a tms $(y_\alpha)_{\alpha \in \mathcal{A}}$ such that there exists a flat extension $(z_\beta)_{|\beta| \leq 2k}$ with $2k > d$, $M_k(z) \geq 0$, and $M_{k-d_{g_i}}(g_i \star z) \geq 0$ for $i = 1, \dots, m$.*

D. Semi-definite program and the entanglement problem

For a given tms $(y_\alpha)_{|\alpha| \leq d}$, finding an extension $(z_\beta)_{|\beta| \leq 2k}$ as in the theorem above amounts to constructing a positive matrix $M_k(z)_{\alpha\beta} = z_{\alpha+\beta}$ with some entries given, namely $z_\alpha = y_\alpha$ for $|\alpha| \leq d$, and constraints of positivity of moment matrices and localizing matrices, which are linear in the z_α . This type of problem corresponds to what is known in numerical analysis as semi-definite program (SDP) problems. Here, the variables of the SDP are the z_β for $|\beta| \leq 2k$. The smallest extension order is $k_0 = \lfloor d/2 \rfloor + 1$. All the constraints of Theorem 1 can be directly implemented in the SDP apart from the flatness condition (28). If also the flatness condition could be implemented efficiently then $P = NP$ [19]. To take into account the flatness condition, the idea [17] is to consider the SDP

$$\min_z \sum_{\alpha, |\alpha| \leq k_0} R_\alpha z_\alpha \quad \text{such that} \quad (29)$$

$$M_k(z) \geq 0 \quad (30)$$

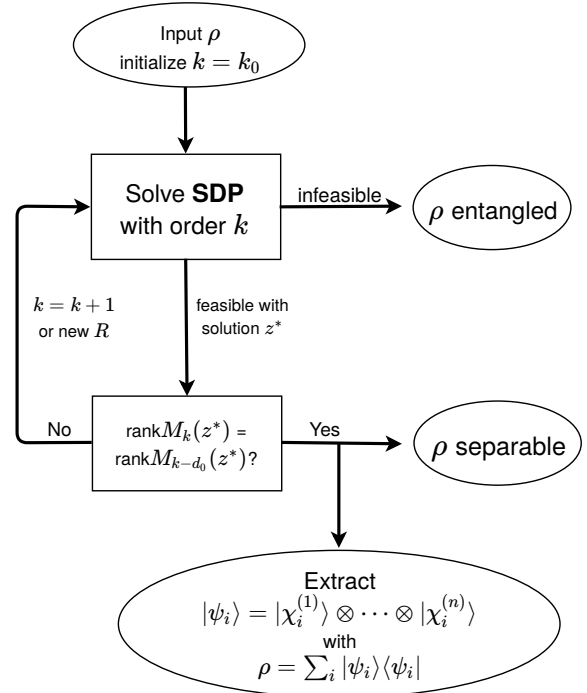
$$M_{k-d_i}(g_i \star z) \geq 0 \quad \text{for } i = 1, \dots, m \quad (31)$$

$$z_\alpha = y_\alpha \quad \text{for } |\alpha| \leq d. \quad (32)$$

The coefficients R_α are chosen randomly, but in order to ensure that $\sum_{\alpha, |\alpha| \leq k_0} R_\alpha z_\alpha$ has indeed a global minimum, the polynomial $R(\mathbf{x}) = \sum_{\alpha} R_\alpha x^\alpha$ is taken as a sum-of-squares polynomial of degree $2k_0$. When the order of the extension k is increased, the polynomial is kept the same, so that minimization is realized only on the z_β with $|\beta| \leq 2k_0$.

According to the theorems above, finding a representing measure, or finding a decomposition into a mixture of separable product states, amounts to finding an extension z that fulfills the constraints (30)–(32), i.e. such that the SDP is "feasible", and that also fulfills the rank condition (28). We can now propose an algorithm which, for any entangled state, provides a certificate of entanglement, and for a separable state usually halts at the first iteration $k = k_0$ and provides a decomposition into pure product states. This algorithm is illustrated in Fig. 1. One runs the algorithm by starting from the lowest possible extension order $k = k_0$ and increasing k . If there exists an order k such that the SDP is infeasible, then the tms y admits no representing measure. In terms of entanglement, this means that the quantum state whose coordinates are given by the y_α is entangled. If, on the contrary, the SDP problem is feasible at some order k (i.e. if all constraints can be met) and if for that value of k the extension obtained fulfills (28), then the tms y admits a representing measure, and the corresponding quantum state is separable with respect to the multipartite factorization of Hilbert space considered. The algorithm remains inconclusive as long as the SDP remains feasible but with an extension which is not flat. In such a case, one can either repeat the SDP with the same k and a different R , or increase the order k by one. As

FIG. 1: Flow diagram to visualize the algorithm. "Solve SDP" refers to (29)–(32)



soon as the rank condition is met, or the SDP becomes infeasible, the algorithm stops and gives a certificate of separability, or entanglement. The only situation where the algorithm does not give an answer in a finite number of steps is the case where extensions are found for any k and all choices of R , but are never flat.

When the algorithm stops with a feasible flat extension z it is possible to extract a representing measure as a sum of $\text{rank}[M_k(z)]$ delta functions [16], which provides an explicit factorization of the separable quantum state. Indeed, suppose the algorithm stops at order k and gives an extension $z = z^*$ which optimizes (29) and fulfills the rank condition (28). If the moment matrix of the optimal solution $M_k(z^*)$ has rank r , then it is possible to calculate an explicit decomposition of the form

$$M_k(z^*)_{\alpha\beta} = \sum_{j=1}^r w_j x^*(j)^\alpha x^*(j)^\beta, \quad |\alpha|, |\beta| \leq k, \quad (33)$$

with $w_j \geq 0$, $\sum_j w_j = 1$, and $\mathbf{x}^*(j) \in K$, with the methods described in [33] and implemented in the Matlab package Gloptipoly 3 [34] (see Appendix A). These r vectors yield r delta functions in the decomposition of the representing measure, and for a separable quantum state they yield an explicit decomposition as a sum of r factorized states.

IV. IMPLEMENTATION AND NUMERICAL RESULTS

A. Two-qubit symmetric states

We now apply this tms approach to some concrete examples of entanglement detection, starting with the simplest case of two-qubit symmetric states. Any state ρ can be expanded as in Eq. (3) with $N = 2$. The tms problem is given by (10) with $d = N = 2$ and $n = 3$ variables. We can choose to obtain a decomposition of the state either into mixed states, in which case the compact K should be taken as the unit ball, or into pure states, where K has to be the unit sphere. Here we consider the pure state decomposition, so that we define $K = \{\mathbf{x} \in \mathbb{R}^3 | g(\mathbf{x}) = 0\}$ with $g(\mathbf{x}) = x_1^2 + x_2^2 + x_3^2 - 1$ (equality $g(x) = 0$ obviously means that K is semi-algebraic and defined by the two polynomials $g \geq 0$ and $-g \geq 0$). The measure $d\mu$ must satisfy constraints such as

$$y_{110} = \int_{\|\mathbf{x}\|=1} x_1 x_2 d\mu(\mathbf{x}) \quad \text{or} \quad y_{002} = \int_{\|\mathbf{x}\|=1} x_3^2 d\mu(\mathbf{x}) \quad (34)$$

where $\|\mathbf{x}\|^2 = x_1^2 + x_2^2 + x_3^2$ and the y_α are the entries corresponding to the $X_{\mu_1 \mu_2}$.

The necessary condition given in Subsection IIIB is positivity of the moment matrix of order $d/2 = 1$, that is, $M_1(y) \geq 0$, with

$$M_1(y) = \begin{pmatrix} y_{000} & y_{100} & y_{010} & y_{001} \\ y_{100} & y_{200} & y_{110} & y_{101} \\ y_{010} & y_{110} & y_{020} & y_{011} \\ y_{001} & y_{101} & y_{011} & y_{002} \end{pmatrix}. \quad (35)$$

Solving the entanglement problem in this case amounts to constructing a tms $(z_\beta)_{|\beta| \leq 2k}$ which is a flat extension of y . Since $k_0 = 2$, the lowest-order moment matrix of the extension is $M_2(z)$, which is a 10×10 matrix whose upper left 4×4 block is the matrix (35). The conditions of Theorem 2 imply that we look for an extension such that $M_2(z) \geq 0$ and $M_1(g * z) \geq 0$, where

$$M_1(g * z) = \begin{pmatrix} z_{000} - z_{200} - z_{020} - z_{002} & z_{100} - z_{300} - z_{120} - z_{102} & z_{010} - z_{210} - z_{030} - z_{012} & z_{001} - z_{201} - z_{021} - z_{003} \\ z_{100} - z_{300} - z_{120} - z_{102} & z_{200} - z_{400} - z_{220} - z_{202} & z_{110} - z_{310} - z_{130} - z_{112} & z_{101} - z_{301} - z_{121} - z_{103} \\ z_{010} - z_{210} - z_{030} - z_{012} & z_{110} - z_{310} - z_{130} - z_{112} & z_{020} - z_{220} - z_{040} - z_{022} & z_{011} - z_{211} - z_{031} - z_{013} \\ z_{001} - z_{201} - z_{021} - z_{003} & z_{101} - z_{301} - z_{121} - z_{103} & z_{011} - z_{211} - z_{031} - z_{013} & z_{002} - z_{202} - z_{022} - z_{004} \end{pmatrix} \quad (36)$$

is the 4×4 localizing matrix of z . The SDP is then to find $\min_z \sum_\alpha R_\alpha z_\alpha$, with R an arbitrary given list of coefficients so that $\sum_\alpha R_\alpha z_\alpha$ is positive and bounded, under the constraints that $M_2(z) \geq 0$, $M_1(g * z) \geq 0$ and $z_\alpha = y_\alpha$ for $|\alpha| \leq 2$.

The point of this subsection was to illustrate the different ingredients of our algorithm. In fact, in this case, the necessary condition $M_1(y) \geq 0$ is necessary and sufficient. Indeed, $M_1(y)$ is exactly the 4×4 matrix $(X_{\mu\nu})_{0 \leq \mu, \nu \leq 3}$, which was proven in [29] to be similar to the partial transpose matrix of ρ up to a factor $1/2$. It is well-known that the partial transpose criterion is a necessary and sufficient separability condition for two qubits [35, 36], hence positivity of $M_1(y)$ suffices to prove separability.

In Theorem 4.7 of [37] the authors solved the K -tms problem of degree 2 in the case where K is defined by a single quadratic equality, by direct proof rather than using the above theorems on generic tms. The key point is a result from [38]. Applying this theorem to a tms y of degree 2 when K is a sphere, the necessary and sufficient conditions for y to admit a representing measure are $M_1(y) \leq 0$ and $y_{000} - y_{200} - y_{020} - y_{002} = 0$. Using the

mapping between the tms problem and the separability problem, this theorem of [37] directly yields the necessary and sufficient condition $M_1(y) \geq 0$ mentioned above for separability of a symmetric two-qubit state (the condition $y_{000} - y_{200} - y_{020} - y_{002} = 0$ being fulfilled for any symmetric two-qubit state). Actually, this problem also coincides with problem of characterizing the convex hull of spin coherent states. For spin-1, a necessary and sufficient criterion was established in terms of positivity of a matrix [39]. Again, this criterion can be shown to coincide with the condition $M_1(y) \geq 0$. Moreover, it was shown in [40] that any separable symmetric two-qubit state could be decomposed as a mixture of four pure product states. The tms approach provides a concise constructive proof of the same fact, as we show in Appendix B.

B. N -qubit symmetric states

The case of an N -qubit symmetric state ρ can be mapped onto the tms problem of Eq. (10) where $\mathbf{x} =$

States \ N	2	3	4	5	6	7	8	9	10	11	12
ρ_{ent}	0.2	0.2	0.4	0.6	1.0	2.1	5.2	11.6	26.8	54.6	170.5
ρ_{sep}	0.7	0.4	0.6	1.0	2.0	4.2	10.2	20.8	66.9	94.5	716.3

TABLE I: Timing of the algorithm in seconds for N -qubit symmetric states as function of N , averaged over 100 random states, when run on a standard desktop PC. The first row corresponds to random states drawn from the uniform Haar measure (following [41]), which are usually entangled. They are typically detected by the condition $M_k(y) \geq 0$. The second row corresponds to random separable states created by randomly mixing random pure separable states. The timing can vary depending on the separable state tested and the randomly generated functional R in (29). Up to six different R are tested before moving to the next order.

(x_1, x_2, x_3) is a vector of \mathbb{R}^3 . We define $K = \{x \in \mathbb{R}^3 | g(\mathbf{x}) = 0\}$, with $g(\mathbf{x}) = x_1^2 + x_2^2 + x_3^2 - 1$ as in the two-qubit case. The highest degree of the monomial x^α in (10) is the total number of indices of the tensor $X_{\mu_1 \dots \mu_N}$, i.e. $d = N$. The degree of the polynomial defining K is 2, and therefore $d_0 = 1$.

To numerically investigate the algorithm for an N -qubit symmetric state we have to solve a SDP with degree $d = N$ and flatness condition $\text{rank} M_k(z) = \text{rank} M_{k-1}(z)$. If the state is entangled (ρ_{ent}) the SDP (29)–(32) should prove infeasible at some value of k , but this usually happens already at the lowest order $k = k_0$. When the state is separable (ρ_{sep}) the algorithm has to find a flat extension for some k , which may require to run the SDP for more than one R , or to increase the values of k . Hence, the run time is typically longer than in the case of an entangled state, as can be seen in Table I. Usually we found a flat extension either at the lowest order $k = k_0$ or at order $k = k_0 + 1$.

C. Physical interpretation of the positivity of $M_k(y)$

Consider a $2k$ -qubit symmetric state ρ . The necessary condition $M_k(y) \geq 0$ of Sec.III B turns out to be equivalent to the positivity of the partial transpose of ρ with respect to the k first qubits. Indeed, let T be the real symmetric matrix defined by

$$T_{\mu, \nu} = X_{\mu_1 \dots \mu_k \nu_1 \dots \nu_k} \quad (37)$$

in terms of the coordinates $X_{\mu_1 \mu_2 \dots \mu_{2k}}$ of ρ [see Eq. (3)], where matrix indices μ and ν are multi-indices $\mu = (\mu_1, \dots, \mu_k)$ and $\nu = (\nu_1, \dots, \nu_k)$, with $0 \leq \mu_i, \nu_i \leq 3$. Then, up to a constant numerical factor, the matrix T is similar to the partial transpose of the density matrix in the computational basis for the partition into two sets of k qubits each [29]. Moreover, T has some recurring rows and columns, which when removed yield exactly the moment matrix $M_k(y)$. A symmetric matrix is positive semi-definite if and only if all principal minors, i.e. the determinant of all submatrices, are non-negative. The determinant of a matrix which has a recurring column

or row is equal to zero, so only the submatrices with non-recurring rows and columns have to be considered. Therefore, T , and thus the partial transpose, is positive semi-definite if and only if the matrix $M_k(y)$ is positive semi-definite. So the necessary condition $M_k(y) \geq 0$ is equivalent to the positive partial transpose criterion of a symmetric state of $2k$ -qubits with equal size partitions. Since for a separable N -qubit state ρ any reduced density matrix of $2k$ qubits has to be separable, the necessary conditions $M_k(y) \geq 0$ with $k \leq N/2$ can be interpreted as positivity of the partial transpose of the reduced density matrices of ρ . This provides an interesting interpretation of the physical meaning of the positivity of the moment matrix.

D. Minimal number of pure product states needed

If a quantum state is separable it can be written as a convex sum of product states. Replacing each product state by its eigenvalue-eigenvector decomposition we obtain a decomposition of the initial quantum state as a convex sum of pure product states. What is the minimal number r_{\min} of pure product states required to decompose an arbitrary separable state?

The answer is unknown in the general case. For symmetric states, pure states in the decomposition have to be symmetric themselves (see e.g. Theorem 1 in [29]). As the appendix B shows, and as was obtained in [40], in the case of two qubits, four states are sufficient to represent any separable symmetric state.

The above algorithm yields $\text{rank} M_k(z) = r$ as an upper bound to the number of pure states required to decompose a given quantum state. In order to investigate systematically the number of states required, we generated symmetric separable states by mixing a large number m of random separable symmetric pure states with random weights as

$$\rho_{\text{sep, sym}} = \sum_{i=1}^m w_i (|\psi_i\rangle\langle\psi_i|)^{\otimes N}, \quad (38)$$

with $\sum_i w_i = 1$, and applied the algorithm to the resulting mixed states. When our algorithm stops with a flat extension z such that $\text{rank} M_k(z) = r$, then r is an upper bound on the true minimal number of separable states required to express $\rho_{\text{sep, sym}}$. Indeed, since the extension depends on the random choice of R_α there may be extensions with a smaller rank, as the algorithm does not minimize this rank. Therefore every number $r < m$ obtained should give an upper bound to the actual generic value for r_{\min} . In practice we generated a large list of separable symmetric states with a value of $m = 25$ for $N \leq 6$ and $m = 45$ for $N > 6$ and found a flat extension for each one. The smallest numbers found are reported in Table II.

N	Min r	# min	States tested
2	4	37304	61494
3	6	2410	60641
4	9	1104	174011
5	12	17	174193
6	17	408	153081
7	22	18	16129
8	29	12	16030
9	35	2	10000
10	42	1	10000

TABLE II: The smallest value of r found, which gives an upper bound on the true value r_{\min} of the maximal number of pure states needed to generate every separable symmetric state. In the third column, # min gives the number of states for which the value min r has been reached among the states tested.

V. A NEW SOLUTION TO A PARTICULAR TMS PROBLEM

The mapping presented above not only helps solving the separability problem, but it can also, conversely, shed light on particular tms problems by using results from entanglement theory. We now give an example of such a situation.

One of the best-known results from entanglement

theory is the Peres-Horodecki criterion, which states that 2×2 and 2×3 systems are separable if and only if the partial transpose is positive [35, 36] (PPT-criterion). It has been generalized to the following two statements: If ρ is supported on $\mathbb{C}^2 \times \mathbb{C}^N$ and the rank $r(\rho) = N$ then ρ is separable (Theorem 1 of [42]) and can be written as a convex sum of projectors on N product vectors (Corollary 3a of [42]).

When ρ is fully symmetric, the above characterizations yield the following result:

Theorem 3 ([43]). *Let ρ be a symmetric N -qubit state with positive partial transpose with respect to the first qubit. If $N = 2$ or 3, or if $N > 3$ and $r(\rho) \leq N$, then ρ is fully separable.*

Note that for four qubits there exist entangled symmetric states with a positive partial transpose [44]. As shown in [29], the PPT conditions can be expressed as linear matrix inequalities involving the entries of the tensor $X_{\mu_1 \mu_2 \dots \mu_N}$, or equivalently the y_α . Rewriting the above theorem for $N = 3$ in the language of K -tms problems, this yields a theorem for a special case of a tms. Even more, by using the fact that 2×3 systems are separable if and only if they are PPT, we directly get a necessary and sufficient condition for a tms problem of degree $d = 3$ to admit a representing measure supported on the unit sphere of \mathbb{R}^3 . This condition reads

$$\left(\begin{array}{cccccccc} y_{000} + y_{001} & y_{100} - iy_{010} & y_{100} + y_{101} & y_{200} - iy_{110} & y_{010} + y_{011} & y_{110} - iy_{020} & y_{001} + y_{002} & y_{101} - iy_{011} \\ y_{100} + iy_{010} & y_{000} - y_{001} & y_{200} + iy_{110} & y_{100} - y_{101} & y_{110} + iy_{020} & y_{010} - y_{011} & y_{101} + iy_{011} & y_{001} - y_{002} \\ y_{100} + y_{101} & y_{200} - iy_{110} & y_{200} + y_{201} & y_{300} - iy_{210} & y_{110} + y_{111} & y_{210} - iy_{120} & y_{101} + y_{102} & y_{201} - iy_{111} \\ y_{200} + iy_{110} & y_{100} - y_{101} & y_{300} + iy_{210} & y_{200} - y_{201} & y_{210} + iy_{120} & y_{110} - y_{111} & y_{201} + iy_{111} & y_{101} - y_{102} \\ y_{010} + y_{011} & y_{110} - iy_{020} & y_{110} + y_{111} & y_{210} - iy_{120} & y_{020} + y_{021} & y_{120} - iy_{030} & y_{011} + y_{012} & y_{111} - iy_{021} \\ y_{110} + iy_{020} & y_{010} - y_{011} & y_{210} + iy_{120} & y_{110} - y_{111} & y_{120} + iy_{030} & y_{020} - y_{021} & y_{111} + iy_{021} & y_{011} - y_{012} \\ y_{001} + y_{002} & y_{101} - iy_{011} & y_{101} + y_{102} & y_{201} - iy_{111} & y_{011} + y_{012} & y_{111} - iy_{021} & y_{002} + y_{003} & y_{102} - iy_{012} \\ y_{101} + iy_{011} & y_{001} - y_{002} & y_{201} + iy_{111} & y_{101} - y_{102} & y_{111} + iy_{021} & y_{011} - y_{012} & y_{102} + iy_{012} & y_{002} - y_{003} \end{array} \right) \geq 0. \quad (39)$$

(see the expression of [29] which explicitly gives the PPT criterion for 3 qubits). This result does not appear to have been known previously in the tms literature.

While (39) is a necessary and sufficient condition in the case of a tms of degree $N = 3$, Theorem 3 also provides us with a sufficient condition for a tms of arbitrary degree N . Indeed, suppose one wants to know whether a given tms y of degree $N > 3$ admits a representing measure on the unit sphere. Using the mapping inverse to the one in Sec.IV B one can construct the density matrix ρ associated with the tms via (3). If ρ is PPT and has rank

$r(\rho) \leq N$, then there exists a representing measure.

VI. CONCLUSIONS

We have proposed a new and elegant solution of the entanglement problem by mapping it to the truncated K -moment problem. Benefiting from the mathematically well-developed field of the theory of moments, we provide an algorithm that for an entangled state certifies its entanglement in a finite number of steps. If the state is separable, it usually halts at the first iteration ($k = k_0$

in Fig.1) and then returns an explicit decomposition of the state into a convex sum of product states. Similarly to previous algorithms, our algorithm makes use of semi-definite programming and “extensions”, but there are a number of conceptual differences that allow us express and solve the problem very elegantly and adapt it easily to different physical situations, including subsystems of different dimensions or symmetries, or incomplete data.

In our approach, rather than working directly with the density matrix, the semi-definite optimization problem is based on moment matrices and localizing matrices, where the latter incorporate the constraints of the states of the sub-spaces. This is possible since these states in the sub-spaces are restricted to compact sets characterized by polynomial constraints (e.g. to Bloch spheres in the case of individual spins-1/2). Both the moment matrix and the localizing matrices must be positive semi-definite for a state to be separable. Extensions are extensions of the moment matrix, and we need not impose a particular symmetry on such an extension, nor positivity of the partial transpose of the state, since this is taken care of by positivity of the moment matrix (see Sec.IV C).

Our algorithm contains in addition a crucial element, namely the idea of “flat extensions”: if at a given order k of the extension the SDP is feasible, one checks whether the rank of the extended moment matrix is the same as the one at order $k - d_0$ [with d_0 related to the largest degree of the constraint polynomials, see after eq.(28)]. If so, the state is separable and one obtains its explicit convex decomposition into product states. In [25] it was already noted that when PPT is imposed on the extensions in the algorithm by Doherty et al. [20–22], *sometimes* separability can be concluded in a finite number of steps by checking whether the rank of the found extension of the density matrix has not increased compared to the original state, a situation called “rank loop”. There, the sufficiency of a rank loop for separability follows from a theorem due to Horodecki et al. [32], according to which a PPT state is separable if its rank is smaller or equal than the rank of the reduced state. In our case, the implementation of the flat-extension query is a decisive part of the algorithm, based on Theorem 1.

Formulating the entanglement as a truncated K -tms problem also has the advantage that the algorithm readily accepts incomplete data from an experiment. Indeed, since for multi-partite systems fully determining the state requires an effort that grows exponentially with the number of subsystems, fully specifying or experimentally determining the state becomes at some point impossible in practice. Since our algorithm is based from the very beginning on a truncated sequence of moments (that can be chosen to be expectation values of Hermitian operators that *were* measured), we can leave open additional moments that were not measured and still run the algorithm. Using the algorithm in this

way should allow one to determine how many and which moments one should measure in order to still be able to prove that a state is entangled.

Finally, as symmetric states of N qubits coincide with spin- j states with $N = 2j$, separable symmetric states can be identified with classical spin- j states (see e.g. [39]). The latter, defined in [39], are convex combinations of spin-coherent states, and can be considered the quantum states which are closest to having a classical behaviour in the sense of minimal quantum fluctuations [13, 29, 45]. Applying the algorithm presented here to symmetric states of N -qubits also allows one to check whether a spin- j state is classical.

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Appendix A: Matlab implementation

Here we give a Matlab implementation of the easiest case of the symmetric state of two qubits, (or a spin-1 state [46]). The quantum state ρ is given as in (2) as

$$X_{\mu_1\mu_2} = \text{tr}\{\rho P_s^\dagger \sigma_{\mu_1} \otimes \sigma_{\mu_2} P_s\}, \quad (\text{A1})$$

with P_s the projector onto the symmetric states. The following implementation uses Matlab and the programs GloptiPoly 3 [34] and the solver SeDuMi [47]. To increase the probability of finding a flat extension, the semi-definite solver should use the highest possible accuracy in the calculation of the minimal value of the SDP.

```

1 mpol x 3
2 xMom=[1 x(1) x(2) x(3) x(1)^2 x(1)*x(2)
        x(1)*x(3) x(2)^2 x(2)*x(3) x(3)^2];
3 y=[X(1,1) X(1,2) X(1,3) X(1,4) X(2,2) X
     (2,3) X(2,4) X(3,3) X(3,4) X(4,4)];
4 con=[mom(xMom)=y];
5 K = [x(1)^2+x(2)^2+x(3)^2-1==0];
6 G = randn(length(xMom));
7 R = xMom*(G'*G)*xMom'; k=2;
8 P = msdp(min(mom(R)),K,con,k);
9 pars.eps=0; mset(pars);
10 [status]=msol(P);

```

Line 3 is given by Eq. (A1). Line 4 corresponds to Eq.(10). K fixes the variables to Bloch vectors of length 1. R is the arbitrary positive bounded polynomial which should be minimized. At line 8, ‘msdp’ formulates the problem in the language of SDPs (construction of moment matrices and localizing matrices). Line 9 sets the

accuracy of the SDP solver to its highest value. At line 10, 'msol' solves the SDP.

- If the problem is detected as infeasible (status=-1) the state is entangled.
- If there is no flat extension found (status=0), one can re-run the program with a different R, or increase the order by one.
- If the state is separable and a flat extension is found (status=1) the solution can be extracted with the command "sol=double(x)". Then "sol" contains a list of Bloch vectors of the pure states that give a decomposition into separable states as in Eq. (6). The vector of weights w_i can then be easily calculated.

This implementation can be extended to a larger number of qubits by adapting the monomial basis in line 2 to a higher degree and line 3 to contain all entries of the tensor $X_{\mu_1 \dots \mu_N}$ (Eq. (2)). The generalization to non-symmetric states is also possible, but the number of variables increases. E.g. two qubits would require one independent Bloch vector for each subsystem, so one would need six variables in total.

Appendix B: Minimal rank for symmetric two-qubit states

Theorem 4.7 of [37] states that a tms y of degree 2 admits a representing measure supported by K if and only if $M_1(y)$ is positive and $y_{000} - y_{200} - y_{020} - y_{002} = 0$. We therefore obtain that a two-bit symmetric state ρ is separable if and only if it is associated with a tms such that $M_1(y)$ is positive and $y_{000} - y_{200} - y_{020} - y_{002} = 0$. These two conditions in fact coincide respectively with the PPT criterion (see Sec.IV C) and with the condition that $X_{00} = \sum_{a=1}^3 X_{aa}$. The latter condition itself is a consequence of properties of the projections of tensor products of Pauli matrices over the symmetric subspace, as was shown in [13].

The proof of the fact that iff $M_1(y)$ is positive and $y_{000} - y_{200} - y_{020} - y_{002} = 0$ then ρ is separable into a mixture of only 4 separable states can be simplified by using the tms formalism. Let us derive the necessary and sufficient condition above in our language. The 'necessary' direction is obvious. The proof for the 'sufficient'

direction goes as follows. Let us assume that the coordinates $X_{\mu\nu}$ form a positive rank- r matrix $M_1(y)$. Since the state is symmetric, $M_1(y)$ is a real symmetric 4×4 matrix and hence $r \leq 4$. Then $M_1(y)$ can be decomposed into a sum of r projectors on orthogonal vectors $u^{(k)}$ as

$$X_{\mu\nu} = \sum_{k=1}^r u_{\mu}^{(k)} u_{\nu}^{(k)}. \quad (\text{B1})$$

Let $\Delta_u = (u_0)^2 - \sum_{a=1}^3 (u_a)^2$ for any 4-vector u . Since $X_{\mu\nu}$ verify $X_{00} = \sum_{a=1}^3 X_{aa}$ we have $\sum_{i=1}^r \Delta_{u^{(i)}} = 0$. Whenever $\Delta_{u^{(i)}} = 0$, one has $u_0^{(i)} \neq 0$ (otherwise the whole vector $u^{(i)}$ vanishes and does not contribute to the sum (B1)), so that the corresponding projector can be rewritten

$$u_{\mu}^{(i)} u_{\nu}^{(i)} = \left(u_0^{(i)}\right)^2 n_{\mu}^{(i)} n_{\nu}^{(i)} \quad (\text{B2})$$

with $n^{(i)} = (1, \mathbf{n})$ and $|\mathbf{n}| = 1$. If all $\Delta_{u^{(i)}} = 0$ then Eqs. (B1)–(B2) immediately yield a sum over r separable pure states. If not, then since $\sum_i \Delta_{u^{(i)}} = 0$ there must be two indices i and j with $\Delta_{u^{(i)}} < 0$ and $\Delta_{u^{(j)}} > 0$. Let $v(t) = tu^{(i)} + (1-t)u^{(j)}$. Then $\Delta_{v(0)} > 0$ and $\Delta_{v(1)} < 0$, so that there has to be a $t_c \in]0, 1[$ such that $\Delta_{v(t_c)} = 0$. The vector $v'(t) = -(1-t)u^{(i)} + tu^{(j)}$ is then such that

$$u_{\mu}^{(i)} u_{\nu}^{(i)} + u_{\mu}^{(j)} u_{\nu}^{(j)} = \frac{v(t_c)_{\mu} v(t_c)_{\nu} + v'(t_c)_{\mu} v'(t_c)_{\nu}}{t_c^2 + (1-t_c)^2}. \quad (\text{B3})$$

Then subtracting a projector on $v(t_c)$ yields

$$X_{\mu\nu} - \frac{v(t_c)_{\mu} v(t_c)_{\nu}}{t_c^2 + (1-t_c)^2} = \sum_{k=1}^{r-1} \tilde{u}_{\mu}^{(k)} \tilde{u}_{\nu}^{(k)} \quad (\text{B4})$$

where $\tilde{u}^{(k)}$ are the orthogonal states $u^{(k')}$ ($k' \neq i, j$) and $v'(t_c)$. Because of the definition of t_c and using (B2), the projector on $v(t_c)$ is proportional to a projector representing a separable pure state, and the remaining sum is such that $\sum_{k=1}^{r-1} \Delta_{\tilde{u}^{(k)}} = 0$. We are therefore back to the form (B1) but with the rank reduced by one. The same procedure can be applied repeatedly to further reduce the rank down to 1; the last projector is then necessarily of the form (B2). In the end, ρ is written as a sum of $r \leq 4$ projectors on separable pure states.

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