Classicality of spin states

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We extend the concept of classicality in quantum optics to spin states. We call a state "classical" if its density matrix can be decomposed as a weighted sum of angular momentum coherent states with positive weights. Classical spin states form a convex set $\mathcal{C}$, which we fully characterize for a spin–1/2 and a spin–1. For arbitrary spin, we provide "non-classicality witnesses". For bipartite systems, $\mathcal{C}$ forms a subset of all separable states. A state of two spins–1/2 belongs to $\mathcal{C}$ if and only if it is separable, whereas for a spin–1/2 coupled to a spin–1, there are separable states which do not belong to $\mathcal{C}$. We show that in general the question whether a state is in $\mathcal{C}$ can be answered by a linear programming algorithm.

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I. INTRODUCTION

The question of the classicality of quantum states has regained interest with the rise of quantum information theory [1]. Stronger–than–classical correlations between different systems are an important resource for quantum communication protocols, and the existence of large amounts of entanglement has been shown to be necessary for a quantum computational speed-up [2, 3]. However, even for a single system the question of classicality is important. Historically the question goes back to two seminal papers in quantum optics by Sudarshan and Glauber [4, 5], who introduced the Glauber–Sudarshan P–representation for the states of a harmonic oscillator. This representation allows to decompose the density matrix in terms of coherent states of the harmonic oscillator. For a single coherent state, the weight function of the P–representation (called P–function in the following for short) reduces to a delta function on the phase space point in which the coherent state is centered, and the dynamics of the P–function is exactly the one of the classical phase space distribution. It has therefore become customary in quantum optics to consider states with a positive P–function as classical. Several other criteria can be derived from this requirement. Using Bochner's theorem for the Fourier transform of a classical probability distribution [6], Richter and Vogel derived a hierarchy of observable criteria based on the characteristic function, which are both necessary and sufficient for classicality [7]. This led to a recent demonstration of the negativity of the P–function in a quantum optical experiment [8]. Korbicz *et al.* realized a connection of the positivity of the P–function to Hilbert's 17th problem of the decomposition of a positive polynomial [9]. Since the P–function for a continuous variable system can be highly singular, a lot of attempts to define classicality have been based on other quasi-probability distributions [10] as well, notably the Wigner function [11, 12].

These quasiprobability distributions for the harmonic oscillator [10] have analogs for finite–dimensional angular momentum states [13]. The Wigner function for finite–dimensional systems has received a large amount of attention, ranging from questions of its most appropriate definition [13, 14, 15, 16, 17], over classicality criteria [18, 19], to the importance of its negativity for quantum computational speed-up [20] (see also for further references concerning the historical development of the Wigner function for finite–dimensional systems). Surprisingly, the P–function for finite–dimensional systems has been much less studied, in spite of its attractive mathematical properties. The P–function for a system with a finite–dimensional Hilbert space (i.e. formally a spin system) allows to decompose the density matrix in terms of angular momentum coherent states [21]. It can always be chosen to be a smooth function, expandable in a finite set of spherical harmonic functions [13]. In contrast to the case of the harmonic oscillator, questions concerning the existence of the P–function (or its nature as a distribution or worse) do therefore not arise. This idyllic situation is somewhat perturbed, however, by the fact, already observed in [21], that for a spin system a large amount of freedom exists in the choice of the P–function, as it depends on two continuous variables on the Bloch sphere, whereas the density matrix for a system with d–dimensional Hilbert space is specified by $d^2 - 1$ real independent entries.

In this paper we show that the existence of a P–representation of the state of a spin system with a positive P–function is a meaningful concept which allows to define the classicality of states of finite–dimensional systems in a natural fashion, completely analogous to the classicality of the harmonic oscillator states of the electromagnetic field. We shall call the corresponding states "P–representable", or P–rep for short. The set $\mathcal{C}$ of P–representable states form a convex domain in the space of density operators, containing the completely mixed state in its interior. We show that, surprisingly, all states of a single spin–1/2 are P–rep, and obtain an analytical criterion for P–representability in the case of a spin–1. For bipartite systems, the set of P–rep states is a subset of the set of separable states. For two spins–1/2 the two sets coincide, whereas already for a spin–1/2 combined with a spin–1, there are separable states which are not P–rep. We also show that the problem of deciding whether a given state is P–rep can be solved numerically by linear programming.

In the following we will first motivate and define P–representability, then study simple cases of small spins, introduce a variational approach that gives rise to a linear programming algorithm, and finally have a look at composite systems. We also develop some necessary conditions for P–representability based on measurable observables, which may thus serve as "non–classicality witnesses", an extension of the by now well-known concept of entanglement witnesses [22].

II. DEFINITION OF P–REPRESENTABILITY

A. Coherent states

We first set some notations following the lines of [13]. Angular momentum coherent states are defined as eigenstates of $\mathbf{J}^2$ and $\mathbf{n}.\mathbf{J}$ with eigenvalues $j(j+1)$ and j, respectively, where $\mathbf{n}$ is a unit column vector which specifies the quantization axis with polar angle θ and azimuth φ, and $\mathbf{J}$ is the familiar angular momentum operator with components J_x, J_y and J_z. The transpose of the column vector $\mathbf{n}$ reads

$$\mathbf{n}\left(\theta,\varphi\right)^t = \left(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\right).$$

An angular momentum coherent state can be expanded in terms of the states $|jm\rangle$ quantized on the z axis as

$$\begin{aligned}|\theta\varphi\rangle &= \sum_{m=-j}^{j}\sqrt{\binom{2j}{j+m}} \\ &\times \left(\sin\frac{\theta}{2}\right)^{j-m}\left(\cos\frac{\theta}{2}\right)^{j+m} e^{-i(j+m)\varphi}\,|jm\rangle\,.\end{aligned}$$

The coherent states form a complete, although not orthogonal, basis set of normalized states within the space of the eigenfunctions of $\mathbf{J}^2$ with given j, and

$$\frac{2j+1}{4\pi}\int \sin\theta d\theta d\phi\,|\theta\varphi\rangle\langle\theta\varphi| = \mathbf{1}_{2j+1}, \qquad (1)$$

where $\mathbf{1}_{2j+1}$ is the $(2j+1)$–dimensional identity matrix. We shall use the shorthand $\alpha = (\theta,\varphi)$ and denote $d\alpha = \sin\theta d\theta d\phi$. The coherent state $|\theta\varphi\rangle$ associated with the vector $\mathbf{n}$ will be denoted $|\mathbf{n}\rangle$ or $|\alpha\rangle$.

B. P–representation

The P–representation of a density operator ρ is an expansion over the overcomplete basis of coherent states. This expansion reads

$$\rho = \int d\alpha P\left(\alpha\right)|\alpha\rangle\langle\alpha|\,, \qquad (2)$$

where the P–function $P\left(\alpha\right)$ is real and normalized by the condition

$$\mathrm{tr}\rho = \int d\alpha P\left(\alpha\right) = 1\,. \qquad (3)$$

If $P\left(\alpha\right)$ is non-negative then ρ is a classical mixture of pure coherent states with probability density $P\left(\alpha\right)$, and can therefore be considered as classical. In this case we shall say that ρ is P–representable, or "P–rep" for short.

This definition has to be made more precise considering that $P(\alpha)$ is not uniquely determined by the density operator. To show this, consider the multipole expansion of ρ,

$$\begin{aligned}\rho &= \sum_{K=0}^{2j}\sum_{Q=-K}^{K}\rho_{KQ}\widehat{T}_{KQ}, \qquad \rho_{KQ} = \mathrm{tr}\rho\widehat{T}_{KQ}^{\dagger}, \qquad (4)\\ \hat{T}_{KQ} &= \sum_{m_1,m_2}^{j}(-1)^{j-m+Q}C_{jm_1jm_2}^{KQ}\,|jm_1\rangle\langle jm_2| \qquad (5)\end{aligned}$$

where $C_{jm_1jm_2}^{KQ}$ are the Clebsch-Gordan coefficients as [23]. Expanding the P–function as a sum of spherical harmonics,

$$P(\alpha) = \sum_{K=0}^{\infty}\sum_{Q=-K}^{K}P_{KQ}Y_{KQ}(\alpha),$$

one obtains a one-to-one relation between the coefficients of the two expansions for $0 \leq K \leq 2j$,

$$\rho_{KQ} = P_{KQ}\sqrt{4\pi}\frac{(2j)!}{\sqrt{\Gamma(2j-K+1)\Gamma(2j+K+2)}}. \qquad (6)$$

If $K > 2j$ the Euler Gamma functions in the denominator become infinite; consequently regardless of P_{KQ} the respective ρ_{KQ} will be zero. It means that the choice of such P_{KQ} is totally arbitrary. However, non-negativity of a $P(\alpha)$ for one choice of P_{KQ} with $K > 2j$ may be absent for another choice. Here is a simple example. Let the density operator be a projector on a coherent state, $\rho = |\alpha_0\rangle\langle\alpha_0|$. An obvious P-function in this case is $\delta(\alpha-\alpha_0)$; it can be considered non-negative since it can be approached by a sequence of non-negative functions, like Gaussians with decreasing width. An alternative choice however would be to drop all non-physical terms in P with $K > 2j$, replacing the δ-function by a finite linear combination

$$P(\alpha) = \sum_{K=0}^{2j}\sum_{Q=-K}^{K}Y_{KQ}^{*}(\alpha_0)Y_{KQ}(\alpha)$$

which is *not* non-negative for all finite j (its tail away from the maximum at $\alpha = \alpha_0$ oscillates around zero).

In view of the non-uniqueness of $P(\alpha)$ we reformulate the definition of P–representability demanding that the condition $P \geq 0$ must be fulfilled *at least for one* particular $P(\alpha)$. Under this definition the pure coherent state $\rho = |\alpha_0\rangle\langle\alpha_0|$ will be P–rep, which is intuitively reasonable. We are thus led to the following definition:

Definition 1 *A density matrix ρ is called P–rep if it can be written as a convex sum of coherent states, i.e. as in Eq.* (2) *with a non-negative function $P(\alpha)$.*

We will now derive some simple consequences of this definition.

C. Consequences

Let $\mathcal{V}$ be the vector space of $(2j+1)\times(2j+1)$ hermitian matrices. The scalar product $\langle X, Y\rangle = \mathrm{tr}X^\dagger Y$ defines an operator norm $||X|| = \sqrt{\mathrm{tr}X^\dagger X}$ on $\mathcal{V}$. We denote by $\mathcal{N}$ the subset of non-negative density matrices, and by $\mathcal{C}$ the subset of P–rep states. The boundaries of these sets are respectively denoted $\partial\mathcal{N}$ and $\partial\mathcal{C}$. The following statements follow immediately from the above definition:

1. The totally mixed state $\rho_0 \equiv \frac{1}{2j+1}\mathbf{1}_{2j+1}$ is P–rep, which is readily seen from Eq. (1) taking $P(\alpha) = 1/4\pi$.

2. The set $\mathcal{C}$ of P–rep states is the convex hull of the set of coherent states. In particular, it is a convex set.

3. Since all P–rep states are non-negative (but not vice versa) we have $\mathcal{C} \subseteq \mathcal{N} \subseteq \mathcal{V}$.

4. According to Carathéodory's theorem on convex sets applied to the $(2j+1)^2$–dimensional vector space $\mathcal{V}$, any non-negative Hermitian matrix can be represented as a convex sum of at most $(2j+1)^2+1$ projectors onto coherent states. In the case of density matrices subject to the condition $\mathrm{tr}\rho = 1$ this number is decreased by 1. Finding a P–representation for a state ρ is thus equivalent to finding real non-negative coefficients λ_i and coherent states $|\alpha_i\rangle$ such that

$$\rho = \sum_{i=1}^{(2j+1)^2} \lambda_i |\alpha_i\rangle\langle\alpha_i|. \tag{7}$$

5. A pure state is P–rep if and only if it is a coherent state.
Proof. The "if" part is trivial. For the "only if" part, assume that a state ρ is P–rep, i.e. that there exists a decomposition such as in (7). We have $\mathrm{tr}\rho^2 = \sum_{i,j}\lambda_i\lambda_j|\langle\alpha_i|\alpha_j\rangle|^2 \le \left(\sum_i \lambda_i\right)^2 = 1$, where equality occurs only for $|\langle\alpha_i|\alpha_j\rangle| = 1$ for all i, j. The latter condition can only be fulfilled if there is a single term in the sum. Thus a pure P–rep state, for which $\mathrm{tr}\rho^2 = 1$, has to be a coherent state.

6. Any density matrix can be decomposed as a sum of the totally mixed state ρ_0 and a traceless hermitian operator $\hat\rho$ with trace norm one multiplied by a positive real parameter κ,

$$\rho_\kappa = \rho_0 + \kappa\hat\rho. \tag{8}$$

Since $\mathcal{C}$ is convex, there is, for any given direction $\hat\rho$, an extremal value κ_e of κ such that $\rho_\kappa \in \mathcal{C}$ if $0 \le \kappa < \kappa_e$ and $\rho_\kappa \notin \mathcal{C}$ if $\kappa > \kappa_e$. The states $\rho = \rho_0 + \kappa_e\hat\rho$ form the boundary $\partial\mathcal{C}$ of P–rep states. They belong to $\mathcal{C}$ provided we accept states ρ as P–rep if they can be approximated in the trace norm by a convex sum of coherent states, that is for all $\epsilon > 0$ there exists a positive function $P(\alpha)$ such that $\left|\left|\rho - \int d\alpha P(\alpha)|\alpha\rangle\langle\alpha|\right|\right| < \epsilon$. With this extended definition the set of P–rep states becomes compact. In some directions the boundary $\partial\mathcal{C}$ may touch $\partial\mathcal{N}$, e.g. when $\rho = |\alpha\rangle\langle\alpha|$ is a pure coherent state.

7. $\partial\mathcal{C}$ is separated by a finite distance from the state ρ_0. In other words, all density operators in some finite neighborhood of ρ_0 are P–rep. To show it let us choose $P(\alpha)$ containing only the mandatory components with $K \le 2j$,

$$\begin{aligned} P(\alpha) &= \frac{1}{4\pi} + \hat P(\alpha), \\ \hat P(\alpha) &= \sum_{K=1}^{2j}\sum_{Q=-K}^{K} P_{KQ} Y_{KQ}(\alpha). \end{aligned} \tag{9}$$

The P_{KQ} are bounded since they are related to the coordinates ρ_{KQ} of ρ by (6) and $\mathrm{tr}\rho^2 \le 1$. As the spherical harmonics are bounded on the sphere and (9) is a finite sum, there is an upper bound $\hat P_e$ to the non-trivial part $\hat P(\alpha)$ when ρ and α are varied. Thus, all matrices $\rho_0 + \kappa\hat\rho$ with $\kappa < 1/(4\pi\hat P_e)$ will be P–rep.

III. P–REP FOR SYSTEMS OF SMALL SPIN

In the case of a spin–1/2 or a spin–1, it is possible to obtain a complete characterization of P–rep states.

A. Spin–1/2

We denote by $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ the vector formed by the Pauli matrices. Together with the identity matrix $\mathbf{1}_2$ they form a basis of the space of 2×2 matrices. Any 2×2 Hermitian matrix with unit trace can be written as

$$\rho = \frac{1}{2}\left(\mathbf{1}_2 + \mathbf{u}.\boldsymbol{\sigma}\right), \tag{10}$$

and $\mathbf{u}$ is given by $\mathbf{u} = \mathrm{tr}(\rho\boldsymbol{\sigma})$. The matrix ρ is non-negative if and only if $|\mathbf{u}| \le 1$. A physical density matrix ρ can thus be represented by a point inside the unit sphere (the Bloch sphere). Matrices corresponding to points on the unit sphere are pure states. Since for spin–1/2 any pure state is a coherent state, the convex hull of coherent states is the convex hull of pure states, which is the set of all density matrices. Thus all states are P–rep.

It is straightforward to find an explicit decomposition in terms of angular momentum coherent states by simply diagonalizing ρ, which leads to the sum of two projectors with two positive eigenvalues. Nevertheless, there is a large freedom in choosing the coherent states. According to (7), finding a P–representation for ρ amounts to finding positive real coefficients λ_i and projectors on coherent states $|\alpha_i\rangle\langle\alpha_i| = \frac{1}{2}\left(\mathbf{1}_2 + \mathbf{n}^{(i)}.\boldsymbol{\sigma}\right)$ with $|\mathbf{n}^{(i)}| = 1$ such that $\rho = \sum_i \lambda_i |\alpha_i\rangle\langle\alpha_i|$. Since the σ_i form a basis of the 2×2 density matrices, this is equivalent to finding λ_i and norm-1 vectors $\mathbf{n}^{(i)}$ such that

$$\mathbf{u} = \sum_i \lambda_i \mathbf{n}^{(i)}. \tag{11}$$

This can be trivially achieved e.g. by taking any pair of points on the Bloch sphere such that the line joining these two points contains the point representing $\mathbf{u}$ inside the sphere.

B. Spin–1

Let us now consider a spin–1 density matrix. We shall use the representation

$$\rho = \frac{1}{3}\mathbf{1}_3 + \frac{1}{2}\mathbf{u}.\mathbf{J} + \frac{1}{2}\sum_{a,b=x,y,z}\left(W_{ab} - \frac{1}{3}\delta_{ab}\right)\frac{J_aJ_b + J_bJ_a}{2}, \tag{12}$$

where J_a are matrices of the angular momentum with $j = 1$. The J_a and the $(J_aJ_b + J_bJ_a)/2$, together with the identity matrix $\mathbf{1}_3$, form a basis of the vector space $\mathcal{V}$ of 3×3 hermitian matrices. Inverting relation (12) we obtain

$$u_a = \mathrm{tr}\,(\rho J_a)\,, \quad W_{ab} = \mathrm{Tr}\,\rho\,(J_aJ_b + J_bJ_a) - \delta_{ab}, \tag{13}$$

which shows that $\mathbf{u} \in \mathbb{R}^3$ while W is a 3×3 real symmetric tensor with trace 1. The projector on a coherent state $|\mathbf{n}\rangle$, written in the form (12), reads

$$|\mathbf{n}\rangle\langle\mathbf{n}| = \frac{1}{3}\mathbf{1}_3 + \frac{1}{2}\mathbf{n}.\mathbf{J} + \frac{1}{2}\sum_{a,b=x,y,z}\left(n_an_b - \frac{1}{3}\delta_{ab}\right)\frac{J_aJ_b + J_bJ_a}{2}. \tag{14}$$

According to (7), ρ is P–rep if and only if there exist $\lambda_i > 0$ with $\sum_i \lambda_i = 1$ and coherent states corresponding to vectors $\mathbf{n}^{(i)} \in \mathbb{R}^3$ of length 1 such that

$$\begin{aligned} \sum_i \lambda_i n_a^{(i)} &= u_a, \\ \sum_i \lambda_i n_a^{(i)} n_b^{(i)} &= W_{ab}, \end{aligned} \tag{15}$$

(with a, b running over x, y, z). It turns out that these equations admit a solution – and hence ρ is P–rep – if and only if the real symmetric 3×3 matrix Z with matrix elements

$$Z_{ab} = W_{ab} - u_au_b \tag{16}$$

is non-negative.

Proof. First let us assume that the Eqs. (15) do have a solution. Then Z can be written

$$Z_{ab} = \sum_{i,j}\left(\lambda_i\delta_{ij} - \lambda_i\lambda_j\right) n_a^{(i)} n_b^{(j)}, \tag{17}$$

and for any vector $\mathbf{y} \in \mathbb{R}^3$ we have

$$\mathbf{y}^t Z \mathbf{y} = \sum_i \lambda_i \left(\mathbf{y}.\mathbf{n}^{(i)}\right)^2 - \left(\sum_i \lambda_i \mathbf{y}.\mathbf{n}^{(i)}\right)^2 \geq 0 \tag{18}$$

since the weights $\lambda_i > 0$ sum to 1 and $f(x) = x^2$ is a convex function. Therefore Z is indeed non-negative for all P–rep operators ρ.

Conversely, if $Z \geq 0$, then it is possible to exhibit a decomposition of ρ by finding an explicit solution to Eqs. (15). Let A be such that $Z = AA^t$. If we denote by $\mathbf{t}^{(i)}$ the eight column vectors $(\pm 1, \pm 1, \pm 1)$ obtained from all combinations of the $\pm$ signs, and define

$$\tau_i = -\frac{\mathbf{u}^t A \mathbf{t}^{(i)}}{1 - |\mathbf{u}|^2} + \sqrt{1 + \left(\frac{\mathbf{u}^t A \mathbf{t}^{(i)}}{1 - |\mathbf{u}|^2}\right)^2}, \tag{19}$$

then one can check that a solution to Eqs. (15) is given by

$$\mathbf{n}^{(i)} = \mathbf{u} + \tau_i A \mathbf{t}^{(i)} \tag{20}$$

$$\lambda_i = \frac{1}{4}\frac{1}{1 + \tau_i^2}, \tag{21}$$

which proves that ρ is P–rep.

The necessary and sufficient condition $Z \geq 0$ in the case of spin–1 allows to characterize the boundary $\partial\mathcal{C}$ of P–rep states. Indeed, let us consider a one-parameter family of states as in (8). If $\mathbf{u}$ and W are the vector and matrix corresponding to the expansion (12) of the state $\rho_0 + \hat{\rho}$, then the vector and the matrix associated with $\rho_\kappa = \rho_0 + \kappa\hat{\rho}$ are given by

$$\mathbf{u}_\kappa = \kappa\mathbf{u} \tag{22}$$

$$W_\kappa = \kappa W + \left(\frac{1-\kappa}{3}\right)\mathbf{1}_3,$$

and thus the 3×3 matrix Z_κ associated with ρ_κ reads

$$Z_\kappa = \kappa W + \left(\frac{1-\kappa}{3}\right)\mathbf{1}_3 - \kappa^2\mathbf{u}\mathbf{u}^t. \tag{23}$$

The value $\kappa = \kappa_e$ at which the scaled operator ρ_κ ceases to be P–rep corresponds to the smallest κ for which Z_κ has a zero eigenvalue. Thus κ_e is the smallest solution of the equation $\det Z_\kappa = 0$, and the equation of $\partial\mathcal{C}$ in the vector space $\mathcal{V}$ is

$$\kappa_e^2\mathbf{u}^t\left(\kappa_e W + \frac{1-\kappa_e}{3}\mathbf{1}_3\right)^{-1}\mathbf{u} = 1. \tag{24}$$

This equation gives implicitly the value κ_e for each direction $\hat{\rho}$ in the vector space $\mathcal{V}$. As the examples of spin–1/2 and spin–1 show, the proportion of P–rep matrices among all density operators depends on j.

C. Necessary conditions for higher spins

It is possible to derive more general necessary conditions for P–representability of spin–j states, as follows. Let us denote by $J_{\mathbf{t}} = \mathbf{t}.\mathbf{J}$ the spin operator in direction $\mathbf{t}$. For a coherent state $|\mathbf{n}\rangle$ corresponding to a vector $\mathbf{n}$, the mean values of $J_{\mathbf{t}}$ and $J_{\mathbf{t}}^2$ are given by

$$\langle \mathbf{n}|J_{\mathbf{t}}|\mathbf{n}\rangle = j\ \mathbf{t}.\mathbf{n} \tag{25}$$

$$\langle \mathbf{n}|J_{\mathbf{t}}^2|\mathbf{n}\rangle = \frac{j}{2} + j\left(j - \frac{1}{2}\right)(\mathbf{t}.\mathbf{n})^2 . \tag{26}$$

Any P–rep state ρ can be written as $\rho = \sum_i \lambda_i |\mathbf{n}^{(i)}\rangle\langle\mathbf{n}^{(i)}|$, which implies for the mean values of $J_{\mathbf{t}}$ and $J_{\mathbf{t}}^2$ in the state ρ

$$\langle J_{\mathbf{t}}\rangle = j \sum_i \lambda_i\ \mathbf{t}.\mathbf{n}^{(i)} \tag{27}$$

$$\langle J_{\mathbf{t}}^2\rangle = \frac{j}{2} + j\left(j - \frac{1}{2}\right)\sum_i \lambda_i \left(\mathbf{t}.\mathbf{n}^{(i)}\right)^2 . \tag{28}$$

Convexity of $f(x) = x^2$ applied to the sums over i leads to the inequality

$$2j\langle J_{\mathbf{t}}^2\rangle - (2j-1)\langle J_{\mathbf{t}}\rangle^2 - j^2 \geq 0 \quad \forall \mathbf{t},\ |\mathbf{t}| = 1, \tag{29}$$

with equality if and only if ρ is itself a coherent state. This is a necessary condition for P–rep, valid for any j. In the particular case of spin–1/2 this inequality becomes $\langle J_{\mathbf{t}}^2\rangle \geq 1/4$, which is obviously true for all states ρ and all directions $\mathbf{t}$. In the case of spin–1 the inequality (29) can be rewritten as

$$\sum_{a,b}\left(2\langle J_a J_b\rangle - \langle J_a\rangle\langle J_b\rangle - \delta_{ab}\right) t_a t_b \geq 0 \quad \forall \mathbf{t} = (t_x, t_y, t_z),\ |\mathbf{t}| = 1. \tag{30}$$

As can be seen from Eqs. (13) and (16), this inequality exactly corresponds to the condition $Z \geq 0$ derived in the previous section.

For higher spins, one can similarly derive other necessary conditions. For instance for a P–rep state of spin–3/2, one has

$$\langle J_{\mathbf{t}}^3\rangle = \frac{21}{8}\sum_i \lambda_i \left(\mathbf{t}.\mathbf{n}^{(i)}\right) + \frac{3}{4}\sum_i \lambda_i \left(\mathbf{t}.\mathbf{n}^{(i)}\right)^3 , \tag{31}$$

and a necessary condition imposed by the fact that $|\sum_i \lambda_i x_i^3| \leq \sum_i \lambda_i x_i^2$ for any $x_i \in [-1, 1]$ reads

$$\forall \mathbf{t}, \quad 2\left|\langle J_{\mathbf{t}}^3\rangle - \frac{7}{4}\langle J_{\mathbf{t}}\rangle\right| \leq \left|\langle J_{\mathbf{t}}^2\rangle - \frac{3}{4}\right| . \tag{32}$$

These necessary conditions can be considered as "non-classicality witnesses", as a state ρ is not in $\mathcal{C}$ if at least one of these conditions is not fulfilled.

IV. NUMERICAL IMPLEMENTATION

A. Variational approach to P–representability

Suppose we are given a density operator and want to establish whether it is P–representable. Let us use the multipole expansion (4). The coefficients P_{KQ} with $0 \leq K \leq 2j$ will be defined by Eq. (6). Orthogonality of the spherical harmonics implies that the hypothetical $P(\alpha) \geq 0$ satisfies the integral equations

$$\int P(\alpha) Y_{KQ}^*(\alpha) d\alpha = P_{KQ}, \quad 0 < K \leq 2j, \quad |Q| \leq K, \tag{33}$$

together with

$$\int P(\alpha) d\alpha = \mathrm{tr}\rho = 1.$$

If we find any $P(\alpha) \geq 0$ satisfying these equations the state in question is P–representable.

We can ask for more and try to find the representability boundary for all matrices of the form $\rho_\kappa = \rho_0 + \kappa\hat{\rho}$ obtained by scaling a given traceless normalized hermitian matrix $\hat{\rho}$. To that end, we consider the set of matrices $\rho_0/\kappa + \hat{\rho}$, $\kappa > 0$. These states all have the same traceless part $\hat{\rho}$, thus they are represented by P–functions $P(\alpha)$ that satisfy Eqs. (33) with P_{KQ} corresponding to $\hat{\rho}$, but with $\int P(\alpha) d\alpha = \frac{1}{\kappa}$. We look at the minimum of the functional $F[P] \equiv \int P(\alpha) d\alpha$ over these states. Suppose that the minimum is realized by some function $P_e(\alpha)$ and introduce κ_e through

$$\min \int P(\alpha) d\alpha = \int P_e(\alpha) d\alpha = \frac{1}{\kappa_e}. \tag{34}$$

The corresponding density operator $\rho_{\kappa_e} = \rho_0 + \kappa_e\hat{\rho}$ is represented by the function $\kappa_e P_e(\alpha)$. As we pointed out it means that all operators ρ_κ with $0 \leq \kappa < \kappa_e$ are P–representable and that ρ_e belongs to the boundary $\partial\mathcal{C}$.

B. Concavity of $1/\kappa_e$

The parameter κ_e corresponding to the border of P–rep depends on the matrix ρ, such that $\kappa_e = \kappa_e(\rho)$. Let us take two matrices, ρ^I and ρ^{II} and calculate the respective $\kappa_e(\rho^I)$, $\kappa_e(\rho^{II})$. Consider now a convex combination

$$\rho^{(c)} = c\rho^I + (1-c)\rho^{II}, \quad 0 < c < 1.$$

Then

$$\frac{1}{\kappa_e(\rho^{(c)})} \leq \frac{c}{\kappa_e(\rho^I)} + \frac{1-c}{\kappa_e(\rho^{II})},$$

i.e., $1/\kappa_e$ is a concave function of ρ. The proof is based on Eq. (34). Let P_e^I, P_e^{II} be the functions minimizing $\int P d\alpha$ under constraints corresponding to the operators ρ^I and ρ^{II} respectively. Then the function $P^{(c)} = cP_e^I +$

$(1-c)P_e^{II}$ will obey the constraints corresponding to the operator $\rho^{(c)}$. Therefore we must have

$$\begin{aligned}\frac{1}{\kappa_e(\rho^{(c)})} &= \min\int P(\alpha)\,d\alpha \le \int P^{(c)}(\alpha)\,d\alpha \\ &= c\int P_e^I(\alpha)\,d\alpha + (1-c)\int P_e^{II}(\alpha)\,d\alpha \\ &= \frac{c}{\kappa_e(\rho^I)} + \frac{1-c}{\kappa_e(\rho^{II})},\end{aligned}$$

which implies concavity of $1/\kappa_e$. Thus the knowledge of κ_e for two density matrices gives a lower bound for a whole family of convex combinations of these density matrices.

C. Linear programming

In order to numerically implement the variational approach described here, let us choose the trial P–function in the form of a linear combination of δ-peaks

$$P(\alpha) = \sum_{i=1}^{n} w_i \delta(\alpha - \alpha_i) \tag{35}$$

where the points $\alpha_i = (\theta_i, \phi_i)$ are more or less uniformly distributed on the unit sphere, and $w_i \ge 0$ are non-negative variational parameters; the delta-functions are assumed to be normalized on the unit sphere, $\delta(\alpha - \alpha_i) = \delta(\cos\theta - \cos\theta_i)\,\delta(\phi - \phi_i)$. Inserting this $P(\alpha)$ in (33) we come to the optimization problem: find $\mathbf{w} = \{w_1, \ldots, w_n\}$ with all $w_i \ge 0$, $i = 1 \ldots n$, minimizing the sum

$$F(\mathbf{w}) = \sum_{i=1}^{n} w_i, \tag{36}$$

and subject to $M = (2j+1)^2 - 1$ linear constraints

$$\sum_{i=1}^{n} Y_{KQ}(\alpha_i)\, w_i = P_{KQ}, \quad 0 < K \le 2j, \quad |Q| \le K.$$

This is a problem of linear programming [24]. Its well-known theorem states that whatever the number of unknowns n the minimum of F is realized on a solution containing no more than M non-zero components. This number is one less than predicted by Caratheodory's theorem because the solution is a boundary, not an internal, point of the set of the density matrices P-representable by (35). The minimum found numerically for a given n yields an upper bound on the exact value of $1/\kappa_e$ (Eq. (34)), i.e., the lower bound on the value of the scaling parameter κ at the border of P–rep in $\rho_\kappa = \rho_0 + \kappa\hat{\rho}$.

The linear programming approach was numerically tested and found efficient for moderate values of j. For a given ρ, the minimal value of κ^{-1} diminished fast with the increase of n and was stable. On the other hand, the solution $\mathbf{w}$ changed erratically with the change of n. That was to be expected considering the freedom in the choice of $P(\alpha)$.

V. COMPOSITE SYSTEMS

The definition of classicality can be extended to systems of more than one particle in a natural way. In the present section we shall consider the case of two particles, but the formalism generalizes to an arbitrary number of particles.

A. Classicality for two particles

The P–representation of a density operator in the case of two spins $j_A$and j_B,

$$\rho = \int d^2\alpha_A d^2\alpha_B P(\alpha_A, \alpha_B)\, |\alpha_A\rangle\, |\alpha_B\rangle\, \langle\alpha_A|\, \langle\alpha_B| \tag{37}$$

with $P \ge 0$ is possible for separable states only; consequently P–rep is a sufficient criterion of separability. The partially transposed matrices ρ^{T_A} and ρ^{T_B} are defined in a fixed computational basis $|ij\rangle \equiv |i\rangle_A \otimes |j\rangle_B$ as $\rho^{T_A}_{ij,kl} = \rho_{kj,il}$ and $\rho^{T_B}_{ij,kl} = \rho_{il,kj}$. They are P–rep if and only if ρ is P–rep, and the corresponding P–functions P^{T_A} and P^{T_B} are simply related to the P–function of ρ by $P^{T_A}(\alpha_A, \alpha_B) = P(\tilde{\alpha}_A, \alpha_B)$, $\tilde{\alpha}_A = (\theta_A, -\varphi_A)$, and correspondingly for P^{T_B}. All previously considered equations are reformulated for two spins in a straightforward manner; we shall list them without commenting.

The representation of ρ in terms of products of spherical multipole operators reads

$$\rho = \sum_{K_A=0}^{2j_A} \sum_{Q_A=-K_A}^{K_A} \sum_{K_B=0}^{2j_B} \sum_{Q_B=-K_B}^{K_B} \rho_{K_AQ_A,K_BQ_B} \widehat{T}^A_{K_AQ_A} \widehat{T}^B_{K_BQ_B}, \tag{38}$$

and we have the P–function expanded into products of spherical harmonics,

$$P(\alpha) = \sum_{K_A=0}^{\infty} \sum_{Q_A=-K_A}^{K_A} \sum_{K_B=0}^{\infty} \sum_{Q_B=-K_B}^{K_B} P_{K_AQ_A,K_BQ_B} Y_{K_AQ_A}(\alpha_A) Y_{K_BQ_B}(\alpha_B).$$

The relation between the coefficients of ρ and P is given by

$$\rho_{K_AQ_A,K_BQ_B} = P_{K_AQ_A,K_BQ_B} \times 4\pi\frac{(2j_A)!\,(2j_B)!}{\sqrt{(2j_A-K_A)!(2j_A+K_A+1)!(2j_B-K_B)!(2j_B+K_B+1)!}},$$

and the density operator with a scaled non-trivial part by

$$\rho_\kappa = \rho_0+\kappa\hat{\rho}, \qquad \rho_0 = \frac{\mathbf{1}_{(2j_A+1)\times(2j_B+1)}}{(2j_A+1)(2j_B+1)}.$$

The following variational problem needs to be solved when the boundary of P–representability is to be found: minimize the functional

$$F\left[P\right] = \int d^2\alpha_A d^2\alpha_B P(\alpha_A,\alpha_B)$$

with $P(\alpha_A,\alpha_B)\geq 0$ satisfying the integral equations

$$\int d^2\alpha_A d^2\alpha_B P(\alpha_A,\alpha_B) Y^*_{K_AQ_A}(\alpha_A) Y^*_{K_BQ_B}(\alpha_B) = P_{K_AQ_A,K_BQ_B}\,, \tag{39}$$

where K_A, K_B run from 0 to $2j$ excluding $K_A=K_B=0$, and $|Q_A|\leq K_A, |Q_B|\leq K_B$. If the minimum of F is equal to

$$F_e = \min F = \int d^2\alpha_A d^2\alpha_B P_e(\alpha_A,\alpha_B) \equiv \frac{1}{\kappa_e}\,,$$

then the density operator lying on the boundary of P–representability will be ρ_{κ_e}.

For the numerical implementation, the integrals are now taken over a product of two unit spheres of Alice and Bob. Let us choose the trial P–function as

$$P\left(\alpha_A,\alpha_B\right) = \sum_{i_A=1}^{n_A}\sum_{i_B=1}^{n_B} w_{i_Ai_B}\,\delta\left(\alpha_A-\alpha^A_{i_A}\right)\delta\left(\alpha_B-\alpha^B_{i_B}\right) \tag{40}$$

where n_A points $\alpha^A_{i_A}$ and n_B points $\alpha^B_{i_B}$ are uniformly scattered over the spheres of Alice and Bob, respectively, and $w_{i_Ai_B}\geq 0$ are n_An_B variational parameters. We now solve the linear programming task: minimize

$$F\left(\mathbf{w}\right) = \sum_{i_A=1}^{n_A}\sum_{i_B=1}^{n_B} w_{i_A\,i_B}$$

with $w_{i_A\,i_B}\geq 0$ satisfying $M=(2j_1+1)^2(2j_2+1)^2-1$ linear constraints,

$$\sum_{i_A=1}^{n_A}\sum_{i_B=1}^{n_B} Y^*_{K_AQ_A}(\alpha^A_{i_A})Y^*_{K_BQ_B}(\alpha^B_{i_B})\,w_{i_Ai_B} = P_{K_AQ_A,K_BQ_B}\,.$$

Here K_A, Q_A, K_B, Q_B take all possible values excluding $K_A=K_B=0$. Again, the optimal solution contains no more than M non-zero elements $w_{i_Ai_B}$.

B. Two spins 1/2

Considering that the density operator of a single spin–1/2 is always P–rep it is easy to see that the density operator for a system of two spins is P- rep if and only if it is separable. Consequently, the necessary and sufficient condition of P–rep is given by the Peres-Horodecki theorem [25, 26]. It means that the boundary of P–representability in the family $\rho_\kappa=\rho_0+\kappa\hat{\rho}$ is reached when either ρ_κ or its partial transpose $\rho_\kappa^{T_A}$ ceases to be non-negative. This was checked numerically in the linear programming approach: the minima $1/\kappa_e$ of the functional $F\left[P\right]$ calculated with the matrix ρ and its partial transpose ρ^{T_A} in all cases coincided with each other and agreed with the scaling necessary to shift the smallest eigenvalue of either ρ or ρ^{T_A} to zero. The optimal P was obtained as a combination of $M=15$ coherent states, some of them with very small weights.

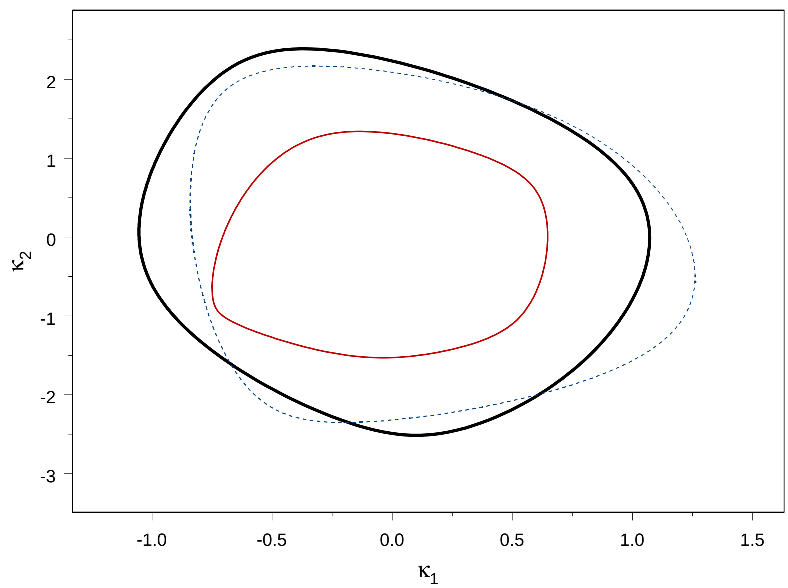

FIG. 1: (Color online) Example of a set of classical states $\mathcal{C}$ for a bipartite system of two spins $1/2$ and 1 parametrized by two parameters, $\rho = \rho_0 + \kappa_1 \hat{\rho}_1 + \kappa_2 \hat{\rho}_2$ with some traceless $\hat{\rho}_1$, $\hat{\rho}_2$. Boundaries are shown of non-negativity of ρ (bold black line), non-negativity of its partial transpose ρ^{T_A} (dashed line), and of P–representability of ρ, ρ^{T_A} (inner red line).

C. Spins 1/2 and 1

In this case the separability and P–rep conditions do not coincide. Indeed consider for instance the pure product state (in $|jm\rangle$ notation) $|\psi\rangle = |\frac{1}{2}\frac{1}{2}\rangle \otimes |10\rangle$. Then the mean value of the operator $\mathbf{1}_2 \otimes J_z^2$ in the state $|\psi\rangle$ is $\langle 10|J_z^2|10\rangle = 0$, while using Eq. (28) one should have for a P–rep state $\langle \mathbf{1}_2 \otimes J_z^2 \rangle \geq 1/2$. Thus, $|\psi\rangle$ is not P–rep. More generally, it is easy to show numerically that $\partial\mathcal{C}$ is well inside the separability boundary. An example is shown in Fig.1, where we display the two boundaries for a density matrix of the form $\rho = \rho_0 + \kappa_1 \hat{\rho}_1 + \kappa_2 \hat{\rho}_2$ with two random but fixed traceless parts $\hat{\rho}_1$ and $\hat{\rho}_2$.

D. Classicality witness

A simple necessary condition for P–rep can be formulated for the density operator ρ of the system of two particles A and B. Let V_A be any non-negative operator in the Hilbert space of A and take the partial trace of ρV_A over the A–variables. Assuming that ρ is P–rep and using the coherent states $|\alpha'\rangle$ for the calculation of the trace we obtain

$$\mathrm{Tr}_A\, \rho V_A = \frac{2j+1}{4\pi} \int d\alpha' \, \langle \alpha' | \rho V_A | \alpha' \rangle \tag{41}$$

$$= \frac{2j+1}{4\pi} \int d\beta \, |\beta\rangle \, \langle \beta| \int d\alpha P(\alpha, \beta) \int d\alpha' \, \langle \alpha | V_A | \alpha' \rangle \, \langle \alpha' | \alpha \rangle \tag{42}$$

$$= \int d\beta \bar{P}(\beta) \, |\beta\rangle \, \langle \beta| \tag{43}$$

where $\bar{P}(\beta) = \int d\alpha P(\alpha, \beta) \langle \alpha | V_A | \alpha \rangle$ is manifestly non-negative. Consequently,

$$\rho_B = (\mathrm{Tr}_A\, \rho V_A) \,/\, \mathrm{Tr}\, \rho V_A \tag{44}$$

can be considered as a density operator in the B–space which is P–representable by a function $\bar{P}(\beta) \,/\, \mathrm{Tr}\, \rho V_A$. Therefore ρ can be P–rep only if ρ_B is also P–rep (not vice versa). The P–rep of ρ_B is easy to check using our result for $j = 1$. One can take, e.g., $V_A = \mathbf{1}_A$ getting $\rho_B = \mathrm{Tr}_A\, \rho$.

VI. CONCLUSION

The P–representable states are classical mixtures of projectors on angular momentum coherent states, i.e. of angular momentum states with minimal uncertainty. The P–rep states have many interesting properties. They can be seen as the "most classical" states, an "inner circle" within the linear space of density operators which forms a convex set $\mathcal{C}$ that contains the totally mixed state in its interior. In the case of two spins, $\mathcal{C}$ is a subset of the set of separable states. The study of the P–representation provides thus important information on the structure of space of density matrices.

We have studied conditions for P–representability, and completely characterized the set of classical states for small spins: for a spin–$1/2$ all states are P–rep, and for a spin–1 we deduced a necessary and sufficient condition for P–rep. In the case of two spins–$1/2$, P–rep is equivalent to separability, but already for a spin–$1/2$ combined with a spin–1, there are states which are separable but not P–rep. In addition, we have shown that the question whether a given state is P–rep or not can be solved with a practical numerical method based on the linear programming algorithm for finding the border of P–rep. We have also formulated necessary conditions based on measurable observables for P–rep, which can be considered "non-classicality witnesses" for spin systems.

Both analytical and computational methods have been used so far on very modest values of j (up to $j \sim 2$); for large j the numerical methods become forbiddingly slow. It would be important to investigate the limit of large j and provide thus a bridge to the case of continuous variables where the P–rep states were an object of intense studies for many years and proved to be of great physical importance.

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[1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, 2000).
[2] R. Jozsa and N. Linden, Proc. R. Soc. Lond. A **459**, 2011 (2003).
[3] G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003).
[4] E. C. G. Sudarshan, Phys. Rev. Lett. **10**, 277 (1963).
[5] R. J. Glauber, Phys. Rev. **131**, 2766 (1963).
[6] S. Bochner, Math. Ann. **108**, 378 (1933).
[7] T. Richter and W. Vogel, Phys. Rev. Lett. **89**, 283601 (2002).
[8] T. Kiesel, W. Vogel, V. Parigi, A. Zavatta, and M. Bellini, arXiv:0804.1016v1.
[9] J. K. Korbicz, J. I. Cirac, J. Wehr, and M. Lewenstein, Physical Review Letters **94**, 153601 (2005).
[10] K. E. Cahill and R. J. Glauber, Phys. Rev. **177**, 1882 (1969).
[11] R. L. Hudson, Rep. Math. Phys. **6**, 249 (1974).
[12] A. Kenfack and K. Życzkowski, J. Opt. B: Quantum Semiclass. Opt. **6**, 396 (2004).
[13] G. S. Agarwal, Phys. Rev. A **24**, 2889 (1981).
[14] J. Hannay and M. V. Berry, Physica D **1**, 267 (1980).
[15] J. P. Dowling, G. S. Agarwal, and W. P. Schleich, Phys. Rev. A **49**, 4101 (1994).
[16] A. M. F. Rivas and A. M. O. de Almeida, Ann. Phys. (N.Y.) **276**, 223 (1999).
[17] P. Bianucci, C. Miquel, J. P. Paz, and M. Saraceno, Phys. Lett. A **297**, 353 (2002).
[18] C. Cormick, E. F. Galvão, D. Gottesman, J. P. Paz, and A. O. Pittenger, Phys. Rev. A **73**, 012301 (2006).
[19] D. Gross, J. Math. Phys. **47**, 122107 (2006).
[20] E. F. Galvão, Phys. Rev. A **71**, 042302 (2005).
[21] F. T. Arecchi, E. Courtens, R. Gilmore, and H. Thomas, Phys. Rev. A **6**, 2211 (1972).
[22] M. Lewenstein, D. Bruss, J. I. Cirac, B. Kraus, M. Kus, J. Samsonowicz, A. Sanpera, and R. Tarrach, J. Mod. Optics **47**, 2841 (2000).
[23] E. Abramowitz and I. A. Stegun, eds., *Handbook of Mathematical Functions* (Dover, 1965).
[24] T. H. Cormen, C. E. Leiserson, R. L. Rivest, and C. Stein, *Introduction to Algorithms*, vol. 2nd edition (MIT Press and McGraw-Hill, 2001).
[25] A. Peres, *Quantum Theory: Concepts and Methods* (Kluwer Academic Publishers, Dordrecht, 1993).
[26] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A **232**, 1 (1996).