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Truncated $\mathfrak{su}(2)$ moment problem for spin and polarization states

Tobias Moroder^{1,2,3}, Michael Keyl⁴ and Norbert Lütkenhaus^{1,2,3}

¹ Quantum Information Theory Group, Institute of Theoretical Physics I,
University Erlangen-Nuremberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

² Max-Planck Research Group for Optics, Photonics and Information, University
Erlangen-Nuremberg, Günther-Scharowsky-strasse 1/Bau 24, 91058 Erlangen, Germany

³ Institute for Quantum Computing, University of Waterloo, 200 University Avenue West,
N2L 3G1 Waterloo, Canada

⁴ Institute for Scientific Interchange Foundation, Quantum Information Theory Unit,
Viale S Severo 65, 10133 Torino, Italy

E-mail: tmoroder@iqc.ca

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Abstract

We address the problem whether a given set of expectation values is compatible with the first and second moments of the generic spin operators of a system with total spin j . Those operators appear as the Stokes operator in quantum optics, as well as the total angular momentum operators in the atomic ensemble literature. We link this problem to a particular extension problem for bipartite qubit states; this problem is closely related to the symmetric extension problem that has recently drawn much attention in different contexts of the quantum information literature. We are able to provide *operational, approximate* solutions for very large spin numbers, and in fact the solution becomes exact in the limiting case of infinite spin numbers. Solutions for low spin numbers are formulated in terms of a hyperplane characterization, similar to entanglement witnesses, which can be efficiently solved with semidefinite programming.

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1. Introduction

The ‘black magic’ calculus of quantum mechanics allows us to make predictions about expectation values of certain measurement outcomes; however, these expectation values are surprising in the following ways: on the one hand we know from Bell’s inequality [1] that not all possible quantum-mechanical expectation values are compatible with a local hidden

variable model; on the other hand, not all expectation values which originate from a non-signaling constrained probability theory are quantum mechanical [2]. Given the quantum-mechanical description of the measurement device, the question arises which expectation values are compatible with quantum theory at all. The quantum-mechanical moment problem [3, 4] as well as its truncated version [4] are famous paradigms of this sort of question. An operational characterization of physical expectation values is of course desirable, however, only few examples are known so far. A well-known example is provided in the context of Gaussian states for systems with finite numbers of degrees of freedom. The first two moments of the corresponding position and momentum operators are compatible with quantum mechanics if and only if the Schrödinger–Robertson uncertainty principle is fulfilled [5]. The condition can be written in terms of the covariance matrix [6], which allows—together with a vector formed by the mean values—an operational low-dimensional description of all the quantum states compatible with the given moments. In most of the literature about Gaussian states this low-dimensional description is exploited, which pinpoints the importance of such a result. By contrast satisfying the Schrödinger–Robertson uncertainty principle is not sufficient to guarantee the existence of a quantum state in the case of higher moments [7], and a straightforward extension of Gaussian states might be non-trivial [8].

Clearly, given a set of linearly dependent operators the corresponding expectation values have to reflect the same linear dependence. In addition, each expectation value has to be in the convex hull of the spectrum of the corresponding operator. In order to exploit further structures of the set of operators, we consider operator sets with an underlying Lie algebra structure. In the following we consider operators which are irreducible representations of the Lie algebra $\mathfrak{su}(2)$, the three-dimensional vector space of all tracefree, 2×2 complex matrices X with $X^\dagger = -X$. The corresponding irreducible representation on the Hilbert space \mathcal{H}_j of dimension $d = 2j + 1$ is denoted by $\partial\pi_j : \mathfrak{su}(2) \rightarrow \mathcal{B}(\mathcal{H}_j)$. In addition, we use the label $\mathcal{L}_k^{(j)} = \partial\pi_j(\sigma_k/2)$ for an irreducible representation of the Pauli operators σ_k , which constitute a basis for the Lie algebra $\mathfrak{su}(2)$. This set of operators satisfies the commutation relations

$$[\mathcal{L}_k^{(j)}, \mathcal{L}_l^{(j)}] = i\varepsilon_{klm}\mathcal{L}_m^{(j)}, \quad (1)$$

where ε_{klm} denotes the Levi-Civita tensor. These commutation relations are well known to be satisfied for the spin operators, and indeed the set of operators $\mathcal{L}_k^{(j)}$ can be considered as the familiar *spin operators* of a total spin j , and we use the term in the following. In fact, the considered scenario appears in a variety of different fields in physics: the macroscopic spin measurements of a state of an ensemble of N two-level atoms only supported on the symmetric subspace are spin operators of a spin $j = N/2$ system [9]; any Stokes operator acting on a two-mode system with fixed total photon number N is described by a similar formalism [10], however in contrast to the spin operators the Stokes operators differ by a factor of 2 in the definition of the commutation relation, hence $\tilde{\mathcal{L}}_k^{(N/2)} = 2\mathcal{L}_k^{(N/2)}$. Note, since there is only one irreducible representation of the Lie algebra $\mathfrak{su}(2)$ in a given, fixed dimension d , the spin operators are unique up to unitary transformations. In addition, the spin operators satisfy the Casimir identity given by

$$(\mathcal{L}_1^{(j)})^2 + (\mathcal{L}_2^{(j)})^2 + (\mathcal{L}_3^{(j)})^2 = j(j+1)\mathbb{1}. \quad (2)$$

In the following, we are interested in the expectation values of products of *two* spin operators only. Although higher moments can be measured in principle, in experiments it is often very tedious to get accurate values for those moments, e.g., [11]. Let us formally denote the set of density operators ρ on a given Hilbert space \mathcal{H} by

$$\mathcal{D}(\mathcal{H}) = \{\rho \in \mathcal{B}(\mathcal{H}) | \rho \geq 0, \text{tr}(\rho) = 1\}. \quad (3)$$

The problem stated below asks for the compatibility of a given set of expectation values with spin operator measurements on a system of fixed dimension⁵.

Problem 1.1 (truncated $\mathfrak{su}(2)$ moment problem). *Consider the set of operators $\mathcal{L}_k^{(j)} \mathcal{L}_l^{(j)}$ with $k, l \in \{1, 2, 3\}$ formed by the products of two spin operators acting on the Hilbert space \mathcal{H}_j with dimension $d = 2j + 1$. Given a set of expectation values $M_{kl} \in \mathbb{C}$ with $k, l \in \{1, 2, 3\}$, under which conditions do these expectation values originate from a quantum-mechanical state, i.e., $\exists \rho \in \mathcal{D}(\mathcal{H}_j)$ such that $\text{tr}(\mathcal{L}_k^{(j)} \mathcal{L}_l^{(j)} \rho) = M_{kl}, \forall k, l$?*

We like to provide an *operational* description of the set of valid expectation values that enables working with the moments directly rather than using the complete density matrix. In order to check for compatibility of a given set of expectation values M_{kl} , the following solution is provided: first, one verifies the linear dependence imposed by the Casimir identity. Next, one reconstructs a particular operator $\rho_j(M)$ which acts on the symmetric subspace of two qubits. The given expectation values are consistent with the spin operators if and only if the operator $\rho_j(M)$ represents a valid density operator for two qubits, which has exactly $2j - 2$ Bose-symmetric extensions. Although this reformulation does not provide an operational description yet, it opens the possibility to apply results from this extension problem directly to problem 1.1. Consequently, one can formulate *operational approximations* to the truncated moment problem. Whenever one finds a separable two qubit state $\rho_j(M)$, then it can be assured that the corresponding expectation values are quantum mechanical, while if one detects non-positivity of a certain operator $\tau_j(\rho_j(M)) \not\geq 0$, that depends on the total spin number j and the reconstructed two-qubit state $\rho_j(M)$, then the expectation values are incompatible with quantum mechanics. This approximate characterization gets more accurate the larger the total spin number j becomes, and converges to the exact solution in the case of infinite spin numbers.

The concept *expectation value matrix* is introduced in section 2, which imposes already a strong condition on quantum-mechanical expectation values in general. The Lie group structure simplifies the problem to a particular standard form of the given expectation value matrix. In section 3, we relate problem 1.1 to the characterization of Bose-symmetric extendible two qubit states by using a particular representation of the spin operators. In addition, we show how this idea directly provides an operational solution to a simplified version of the truncated moment problem. Since the exact solution to this extension problem is unknown, two different methods are considered in order to provide solutions for large (section 4) and small spin numbers (section 5). In particular, section 4 deals with the two different approximation methods which both converge in the limit of high spin numbers. In section 5, a solution to problems of the kind like problem 1.1 in terms of hyperplanes is provided, which can be efficiently solved for low spin numbers j . A graphical comparison between the different sets is given in section 6 that demonstrates already the convergence. In section 7 we summarize and give an outlook on possible further directions.

2. Expectation value matrix

Each expectation value M_{kl} in problem 1.1 is labeled by two indices; therefore, each expectation value constitutes an entry of a particular matrix, which we term *expectation value matrix* in the following. Considering the set of expectation values M in matrix form already enables us to derive a strong statement about quantum-mechanical expectation values

⁵ The considered set of given expectation values stands for knowing the first and second moments of the spin operators in arbitrary directions of the coordinate frame.

in general; it even holds without the Lie group structure and has already appeared in the literature [12–16]. The construction of the expectation value matrix is equivalent to the derivation of the Schrödinger–Robertson uncertainty principle, which all given expectation values must clearly satisfy in order to originate from a quantum state.

2.1. Definition and properties

The expectation value matrix defines a linear map on the set of density operators, which preserves hermiticity and positive semidefiniteness. Therefore every expectation value matrix M , which originates from a valid quantum state ρ , i.e., $M = M(\rho)$, must necessarily be positive semidefinite. The following proposition introduces a slightly bigger *expectation value matrix*⁶ $\chi : \mathcal{B}(\mathcal{H}_j) \rightarrow \mathcal{B}(\mathbb{C}^4)$, which contains our original expectation value matrix M in form of a submatrix, hence the given statements follows automatically. We skip the proof since it has already appeared in the literature, e.g., [13]. Note that further constraints are naturally imposed if the corresponding operator set shows linear dependence. Let us mention that Gaussian states are examples where the conditions on the expectation value matrix are necessary and sufficient for the existence of a quantum state.

Proposition 2.1 (expectation value matrix). *Let \mathcal{F} denote the set of operators acting on the Hilbert space \mathcal{H}_j formed by the identity operator and the spin operators. The expectation value matrix $\chi : \mathcal{B}(\mathcal{H}_j) \rightarrow \mathcal{B}(\mathbb{C}^4)$ is defined by*

$$\mathcal{B}(\mathcal{H}_j) \ni A \mapsto \chi_{kl}(A) = \text{tr}(F_k^\dagger F_l A) \tag{4}$$

with $F_k \in \mathcal{F}$ for $k = 1, \dots, 4$. This expectation value matrix χ has the following properties:

- $\chi(aA + bB) = a\chi(A) + b\chi(B)$ for $A, B \in \mathcal{B}(\mathcal{H}_j)$, $a, b \in \mathbb{C}$.
- If $A = A^\dagger$ then $\chi(A) = \chi(A)^\dagger$.
- If $A \geq 0$ then $\chi(A) \geq 0$.

2.2. Standard form

In order to reduce the number of parameters in the expectation value matrix M we give a *standard form* first. The standard form allows us to consider expectation value matrices with purely imaginary off-diagonal entries only; hence, the set of expectation values is solely characterized by the mean values and the variances of the spin operators $\mathcal{L}_k^{(j)}$. In order to derive the standard form one has to show the covariance property of the expectation value matrix under the adjoint representation of the corresponding Lie group $SU(2)$, given by $\text{Ad} : SU(2) \rightarrow \mathcal{B}(\mathfrak{su}(2))$ and $\text{Ad}_U(x) = U^\dagger x U$, for $U \in SU(2)$ and $x \in \mathfrak{su}(2)$. Acting on the \mathbb{C}^3 , this adjoint representation is unitary equivalent to the irreducible spin-1 representation π_1 of the Lie group $SU(2)$. This allows us to diagonalize the real part of the expectation value matrix. The idea is quite common in the literature of atomic ensembles, see, e.g., [17], hence the proof is omitted.

Proposition 2.2 (covariance property and standard form). *The expectation value matrix $M = M(\rho)$ satisfies the covariance property*

$$M(\pi_j(U) \rho \pi_j(U)^\dagger) = \pi_1(U) M(\rho) \pi_1(U)^\dagger, \quad \forall U \in SU(2) \tag{5}$$

⁶ We use the term *expectation value matrix* for both, the 3×3 matrix M and the 4×4 matrix χ . It should be clear from the context to which matrix one refers.

where π_j denotes the irreducible representation of the group $SU(2)$. Therefore each expectation value matrix M can be transformed to the standard form

$$M = D + iA, \tag{6}$$

where D is a diagonal matrix with fixed trace, $\text{tr}(D) = j(j + 1)$ and iA denotes the anti-Hermitian, tracefree part.

3. Reduction

Each irreducible representation $\partial\pi_j$ of the Lie algebra $\mathfrak{su}(2)$ can be built up from its two-dimensional, fundamental representations $\partial\pi_{1/2}$ by acting on a restricted subspace of the tensor product space of multiple qubits [18]. Such a particular form of the representation appears as the usual representation in the case of atomic ensembles [9]. Given a valid density operator on this restricted tensor product space of multiple qubits, only an effective two qubit state suffices to determine the expectation values of the products of at most *two* Lie algebra elements, cf [19]. Using the prescribed formalism enables us to establish a connection between problem 1.1 and the Bose-symmetric extendibility question for a particular two qubit state, which constitutes the first result. This particular extension problem shows similarities to the so-called symmetric extension problem, which recently has drawn attention in the literature [20–24]. Moreover, we further demonstrate the reduction idea by solving a simplified version of the truncated moment problem.

3.1. Group theory

This part reviews the irreducible representation $\partial\pi_j$ of the Lie algebra $\mathfrak{su}(2)$ on the tensor product space of multiple qubits, restricted to the symmetric subspace. The symmetric subspace $\mathcal{H}_+^{\otimes 2j}$, that is indicated by the subscript +, consists of all vectors $|\psi\rangle \in \mathcal{H}^{\otimes 2j}$, with $\mathcal{H} = \mathbb{C}^2$, that are invariant under all possible permutations $\pi_{2j}(p)|\psi\rangle = |\psi\rangle$, $p \in S_{2j}$. Here π_{2j} denotes an irreducible representation of the permutation group S_{2j} , which acts on a basis formed by product states as given by $\pi_{2j}(p)|i_1\rangle \otimes \dots \otimes |i_{2j}\rangle = |i_{p^{-1}(1)}\rangle \otimes \dots \otimes |i_{p^{-1}(2j)}\rangle$. The following proposition describes the particular form of the representation.

Proposition 3.1 (irreducible $\mathfrak{su}(2)$ representation). *One has:*

- The two Hilbert spaces $\mathbb{C}^{2^{j+1}}$ and $\mathcal{H}_+^{\otimes 2j}$ with $\mathcal{H} = \mathbb{C}^2$ are isomorph.
- The irreducible representation of the Lie algebra $\partial\pi_j : \mathfrak{su}(2) \rightarrow \mathcal{B}(\mathcal{H}_+^{\otimes 2j})$ is given by

$$\partial_j\pi(x) = \sum_{k=1}^{2j} x^{(k)} \Big|_{\mathcal{H}_+^{\otimes 2j}}, \quad x \in \mathfrak{su}(2), \tag{7}$$

with $x^{(k)} = \mathbb{1}^{\otimes k-1} \otimes \partial\pi_{1/2}(x) \otimes \mathbb{1}^{\otimes 2j-k}$, $\partial\pi_{1/2}(x)$ is the two-dimensional fundamental representation and $\Big|_{\mathcal{H}_+^{\otimes 2j}}$ denotes the restriction to $\mathcal{H}_+^{\otimes 2j}$.

3.2. Two qubit reduction

Since the two abstract Hilbert spaces of the previous section are isomorph, any density operator of a spin j system can be interpreted as the density operator of a particular multipartite system of $2j$ qubits, i.e., $\rho_j \in \mathcal{D}(\mathcal{H}_+^{\otimes 2j})$. In the following, we are only interested in the expectation values of products of at most two spin operators. Because of the particular symmetry of the multipartite qubit state and the explicit representation of these operators, these expectation values depend only on an effective spin-1 system. The following proposition summarizes this

reduction and links the corresponding spin operators. This reduction idea already appears in the context of atomic ensembles; a proof can be found, e.g., in [19], which contains also examples of these reduced states.

Proposition 3.2 (spin-1 reduction). *For every density operator $\omega \in \mathcal{D}(\mathcal{H}_+^{\otimes 2j})$, the expectation values of the products of at most two Lie algebra elements only need to be calculated on an effective spin-1 state $\rho_j = \text{tr}_{3\dots 2j}(\omega) \in \mathcal{D}(\mathcal{H}_+^{\otimes 2})$ and are given by $\text{tr}(\partial\pi_j(x)\omega) = \text{tr}(\Lambda(\partial\pi_j(x))\rho_j)$ and similar $\text{tr}(\partial_j\pi(x)^\dagger\partial\pi_j(y)\omega) = \text{tr}(\Lambda(\partial_j\pi(x)^\dagger\partial\pi_j(y))\rho_j)$, for $x, y \in \mathfrak{su}(2)$ with the operators⁷ given by*

$$\Lambda(\partial\pi_j(x)) = (2j\partial\pi_{1/2}(x) \otimes \mathbb{1})|_{\mathcal{H}_+^{\otimes 2}}, \tag{8}$$

for the mean values, and similar for the products of two spin operators

$$\Lambda(\partial\pi_j(x)^\dagger\partial\pi_j(y)) = (2j\partial\pi_{1/2}(x)^\dagger\partial\pi_{1/2}(y) \otimes \mathbb{1} + 2j(2j - 1)\partial\pi_{1/2}(x)^\dagger \otimes \partial\pi_{1/2}(y))|_{\mathcal{H}_+^{\otimes 2}}. \tag{9}$$

Only the reduced spin-1 state $\rho_j = \text{tr}_{3\dots 2j}(\omega)$ of a given multipartite state ω of total spin j determines the expectation values of products of two spin operators. However not all possible spin-1 density operators are actually reduced states of such multipartite states. The formal definition of valid two qubit reductions of a spin j system is given by

$$\mathcal{S}_j = \{ \rho \in \mathcal{D}(\mathcal{H}_+^{\otimes 2}) \mid \exists \omega \in \mathcal{D}(\mathcal{H}_+^{\otimes 2j}), \text{tr}_{3\dots 2j}(\omega) = \rho \}, \tag{10}$$

with $j \geq 1$. Hence, a spin-1 state can correspond to a spin j system if and only if it can be extended to a multipartite state of $2j$ qubits which has support only on the symmetric subspace. This definition resembles the notion of *Bose-symmetric extensions* for bipartite states, which is closely related to the symmetric extensions for bipartite states⁸, cf [20]. The following theorem establishes the connection between the problem 1.1 and the problem of Bose-symmetric extensions of a particular spin-1 state.

Theorem 3.1 (Bose-symmetric extensions \Leftrightarrow quantum-mechanical expectation values). *Given the expectation value matrix M the corresponding spin-1 state $\rho_j = \rho_j(M)$ is uniquely determined by*

$$\text{tr}(\Lambda(\mathcal{L}_k^{(j)}\mathcal{L}_l^{(j)})\rho_j) = M_{kl}, \tag{11}$$

for all $k, l \in \{1, 2, 3\}$, and $\Lambda(\cdot)$ is given by equation (9). The given expectation value matrix M is quantum mechanical if and only if $\rho_j(M) \in \mathcal{S}_j$, i.e., the state $\rho_j(M)$ has exactly $2j - 2$ Bose-symmetric extensions.

Proof. It is straightforward to check that the operators given by equation (9) span an operator basis for a generic spin-1 state, hence the corresponding spin-1 state $\rho_j = \rho_j(M)$ is completely determined by the expectation value matrix M . This particular two-qubit state can correspond to a spin j system if and only if it is an element of the class \mathcal{S}_j . \square

⁷ Note, $\Lambda(\cdot)$ is used as a symbol here and should not be interpreted as a map $\Lambda : \mathcal{B}(\mathcal{H}_+^{\otimes 2j}) \rightarrow \mathcal{B}(\mathcal{H}_+^{\otimes 2})$.

⁸ In the definition of symmetric extensions, as given in [20], the corresponding multipartite state must be invariant under the permutation of the individual subsystems, while in the case of *Bose-symmetric* extensions one requires for the multipartite state to have support on the symmetric subspace only. Although both problems are very similar—and in fact, many results can be ‘borrowed’ directly from the symmetric extension case—certain properties differ. For example, every separable, permutation invariant density operator has a symmetric extension to arbitrary many copies, while it does not need to have a Bose-symmetric extension.

3.3. First moment problem

In the present subsection, we briefly discuss a simplified version of the truncated moment problem in which one asks for compatibility of the first moments only. This problem allows an operational solution and highlights again the importance of the reduction idea. It states as follows:

Problem 3.1 (first moment problem). *Consider the set of spin operators $\mathcal{L}_k^{(j)}$ with $k \in \{1, 2, 3\}$ acting on the Hilbert space \mathcal{H}_j of dimension $d = 2j + 1$. Given a set of expectation values $L_k \in \mathbb{R}$ with $k \in \{1, 2, 3\}$, under which conditions do these expectation values originate from a quantum-mechanical state, i.e., $\exists \rho \in \mathcal{D}(\mathcal{H}_j)$ such that $\text{tr}(\mathcal{L}_k^{(j)} \rho) = L_k, \forall k$?*

The operational description of the set of valid expectation values relies on the reduction to a spin-1/2 problem, in analogy to proposition 3.2, and that every valid spin-1/2 state represents a possible reduced state of a particular spin- j state, i.e., each single qubit density operator can be extended to a Bose-symmetric density operator of $2j$ qubits. The following proposition contains the operational solution.

Proposition 3.3 (operational description). *The expectation values $L_k \in \mathbb{R}$ with $k \in \{1, 2, 3\}$ are compatible with the spin operators of a generic spin j system if and only if it holds*

$$\sum_{i=1}^3 L_i^2 \leq j^2. \tag{12}$$

Proof. In analogy to proposition 3.2, it holds that for every spin- j density operator $\omega \in \mathcal{D}(\mathcal{H}_+^{\otimes 2j})$, the expectation values of each Lie algebra element $\partial\pi_j(x)$ need only to be calculated on an effective qubit state $\tilde{\rho}_j = \text{tr}_{2\dots 2j}(\omega)$ and are given by $\text{tr}(\partial\pi_j(x)\omega) = \text{tr}(\tilde{\Lambda}(\partial\pi_j(x))\tilde{\rho}_j)$ with $\tilde{\Lambda}(x) = 2j\partial\pi_{1/2}(x)$. Contrary to the spin-1 case, every qubit state $\tilde{\rho}$ can be extended back to a multipartite state $\omega = \tilde{\rho}^{\otimes 2j}|_{\mathcal{H}_+^{\otimes 2j}}$, i.e., to a density operator of a spin j system with the correct first moments. Thus, the given expectation values L_k only have to form a valid qubit density operator $\tilde{\rho}_j(\{L_k\}) \in \mathcal{D}(\mathcal{H})$. The set of given expectation values L_k uniquely determines the Bloch vector L_k/j of the reduced qubit state $\tilde{\rho}_j$, which is quantum mechanical if and only if equation (12) holds. \square

We close with a discussion about possible solution states to the first moment problem. Given the set of expectation values, any compatible quantum state can be parameterized as $\rho(\mathbf{x}) = \rho_{\text{fix}}(\{L_k\}) + \rho_{\text{open}}(\mathbf{x})$, with a fixed part $\rho_{\text{fix}}(\{L_k\}) = \mathbb{1}/(2j + 1) + \sum_k a_k \mathcal{L}_k^{(j)}$ and $a_k = L_k / \|\mathcal{L}_k^{(j)}\|_2^2$, that is completely determined by the first moments L_k , and an orthogonal open part $\rho_{\text{open}}(\mathbf{x})$, which linearly depends on some open parameters \mathbf{x} , $x_i \in \mathbb{R}$, and which have to be chosen such that $\rho(\mathbf{x}) \geq 0$ forms a valid density operator. Proposition 3.3 guarantees existence of such a set of open parameters \mathbf{x} as long as the given expectation values fulfill equation (12). A special class of solutions constitutes the case in which $\rho_{\text{fix}}(\{L_k\}) \geq 0$ forms already a positive semidefinite operator itself. However, this is the case if and only if $\sum_{i=1}^3 L_i^2 \leq (j + 1)^2/9$, which shows that the open part $\rho_{\text{open}}(\mathbf{x})$ is indeed necessary since it allows compensation of a non-positive fixed part $\rho_{\text{fix}}(\{L_k\}) \not\geq 0$ in certain cases.

4. Approximating sub- and superset

Any solution to the Bose-symmetric extension problem for two qubits constitutes a solution for the $\mathfrak{su}(2)$ moment problem; however, an analytic characterization of those sets appears

cumbersome. Therefore, two *operational approximation* methods to the set of extendible states are described in the following, which allows identification of certain expectation value matrices, that are either quantum mechanical (subset) or not (superset). Both approximating sets converge to the exact set in the limit of infinite numbers of extensions. The subset characterization relies on a result by Doherty *et al* [20], while the supersets depend on the expectation value matrix. Both approximation sets (and the corresponding convergence statements) are given in terms of renormalized expectation values of an expectation value matrix defined by

$$u_k \equiv \frac{\langle \mathcal{L}_k^{(j)} \rangle}{j}, \quad v_k \equiv \frac{\langle (\mathcal{L}_k^{(j)})^2 \rangle}{j(j-1/2)} - \frac{1}{2j-1}, \quad (13)$$

for $k \in \{1, 2, 3\}$. Note that one has only to consider these six expectation values because of the standard form of the expectation value matrix as described by equation (6). More precisely, the parameters v_k determine the diagonal entries of the expectation value, while u_k fixes the anti-Hermitian, tracefree part. These renormalized expectation values have the advantage that the determined spin-1 state $\rho_j(\{u_k, v_k\})$ is independent of the considered total spin number j .

4.1. Approximating subset

The set of separable two qubit states, supported on the symmetric subspace, forms an approximating subset to the set of Bose-symmetric extendible states, independent of the number of extensions. Hence, if a given expectation value matrix M allows the reconstruction of a separable spin-1 state $\rho_j(M)$, then it can be assured that all expectation values in M are quantum mechanical. The set of separable spin-1 states is given by

$$\mathcal{R} = \{\rho \in \mathcal{D}(\mathcal{H}_+^{\otimes 2}) \mid \rho^\Gamma \geq 0\}, \quad (14)$$

where Γ denotes the partial transpose, which is necessary and sufficient to characterize separable states in these low dimensions [25, 26]. The following theorem outlines the properties of this subset. The convergence result is a direct consequence of a corresponding result for states which have symmetric extensions [20]. For a fixed number of photons, any convex combination of polarization states, where all photons are in one optical mode, constitutes physical relevant examples where the qubit density operator is separable. In contrast, any spin squeezed state must have an entangled two qubit density operator [27], as well as certain multiqubit states in the atomic ensemble literature [28].

Theorem 4.1 (approximating subset). *The sets \mathcal{S}_j with $j \geq 1$, and \mathcal{R} given by equations (10) and (14) respectively satisfy:*

- (i) *If $\rho \in \mathcal{R}$, then $\rho \in \mathcal{S}_j, \forall j$. Hence $\mathcal{R} \subseteq \mathcal{S}_j, \forall j$.*
- (ii) *If $\rho \in \mathcal{S}_j$, then $\rho \in \mathcal{S}_{j'}$ with $j' \leq j$. Hence $\mathcal{S}_j \subseteq \mathcal{S}_{j'}$ for $j' \leq j$.*
- (iii) *$\lim_{j \rightarrow \infty} \mathcal{S}_j \equiv \bigcap_j \mathcal{S}_j \subseteq \mathcal{R}$.*

Proof. Any separable density operator $\rho \in \mathcal{R}$ can be written as a convex combination of pure product states. We assume the following decomposition $\rho = \sum_i p_i |\alpha_i\rangle\langle\alpha_i| \otimes |\beta_i\rangle\langle\beta_i|$, where $\{p_i\}$ denotes the probability distribution and $|\alpha_i\rangle, |\beta_i\rangle \in \mathcal{H}, \forall i$. Because of $\rho \in \mathcal{B}(\mathcal{H}_+^{\otimes 2})$, it must hold that $\text{tr}(P_- \rho) = 0$, where $P_- \geq 0$ denotes the projector onto the antisymmetric subspace. Given the particular decomposition into positive semidefinite operators it follows that the trace must vanish for each term, $\text{tr}(P_- |\alpha_i\rangle\langle\alpha_i| \otimes |\beta_i\rangle\langle\beta_i|) = 0, \forall i$, which shows that each $|\alpha_i\rangle \otimes |\beta_i\rangle \in \mathcal{H}_+^{\otimes 2}$. This can be the case iff $|\alpha_i\rangle = |\beta_i\rangle, \forall i$. This allows us to write a

valid Bose-symmetric extension given by $\omega = \sum p_i |\alpha_i\rangle\langle\alpha_i|^{\otimes 2j}$, which then proves the first statement, $\rho \in \mathcal{S}_j$.

The second statement follows trivially. The last point is a direct consequence of theorem 1 in [20], which states that any bipartite mixed states $\rho_{AB} \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$, which has arbitrary many symmetric extensions to one of the subsystems must necessarily be separable. \square

4.2. Approximating superset

Exploiting the characteristics of the expectation value matrix allows us to formulate an approximating superset to the set of extendible states. Any reduced spin-1 state $\rho_j = \text{tr}_{3..2j}(\omega)$ of a given state $\omega \in \mathcal{D}(\mathcal{H}_+^{\otimes 2j})$ allows the computation of the expectation values of a corresponding spin j system via the operator sets $\Lambda(\cdot)$ given by equations (8), (9); in this sense, the expectation values from a spin j system can be ‘recovered’ from the reduced two qubit state. Proposition 4.1 introduces the *reduced expectation value matrix* τ_j , which tries to reproduce a normalized version of the original expectation value matrix χ of the spin j state only from the reduced spin-1 state; renormalization protects against divergence of the expectation values in the limit $j \rightarrow \infty$. It holds that if the two qubit density operator ρ has a valid extension to $2j$ qubits, then one obtains a positive semidefinite operator.

Proposition 4.1 (reduced expectation value matrix). *Let \mathcal{F} denote the set of operators acting on the Hilbert space \mathcal{H}_j formed by the identity and the renormalized spin operators $\mathcal{L}_k^{(j)}/j$. The reduced expectation value matrix of order j , denoted by $\tau_j : \mathcal{B}(\mathcal{H}_+^{\otimes 2}) \rightarrow \mathcal{B}(\mathbb{C}^4)$, is defined as*

$$\mathcal{B}(\mathcal{H}_+^{\otimes 2}) \ni A \mapsto \tau_j(A)_{kl} = \text{tr}(\Lambda(F_k^\dagger F_l)A), \tag{15}$$

with $F_k \in \mathcal{F}$ for $k = 1, \dots, 4$, and the operators $\Lambda(\cdot)$ are given by equations (8), (9). The map is linear and preserves hermiticity. In addition, it holds that if $\rho \in \mathcal{S}_j$ then

$$\tau_j(\rho) \geq 0. \tag{16}$$

The approximating superset consists of all spin-1 states for which the reduced expectation value matrix of order j delivers a positive semidefinite operator, and is denoted by

$$\mathcal{T}_j = \{\rho \in \mathcal{D}(\mathcal{H}_+^{\otimes 2}) \mid \tau_j(\rho) \geq 0\}, \tag{17}$$

for $j \geq 1$. Unlike the subset characterization, any superset depends on the number of considered extensions j . The following theorem lists the properties of the approximating superset. If a given reconstructed spin-1 operator $\rho_j(M)$ is not an element of the class \mathcal{T}_j , then the corresponding expectation values in M are incompatible with quantum mechanics. The supersets converge to the set of separable states in the limit of infinite number of extensions, hence the reduced expectation value matrix delivers an alternative necessary and sufficient entanglement criterion, valid *only* for symmetric two qubit state, but which does not rely on partial transposition. However, in order to prove convergence, we exploit a necessary and sufficient criterion for entanglement of the reduced two qubit state in terms of the expectation values of the spin operators, cf [29], which is derived using the partial transposition.

Theorem 4.2 (approximating superset). *The sets \mathcal{T}_j with $j \geq 1$ satisfy:*

- (i) *If $\rho \in \mathcal{T}_j$, then $\rho \in \mathcal{T}_{j'}$ with $j' \leq j$. Hence $\mathcal{T}_j \subseteq \mathcal{T}_{j'}$ for $j' \leq j$.*
- (ii) *If $\rho \in \mathcal{S}_j$, then $\rho \in \mathcal{T}_j, \forall j$. Hence $\mathcal{S}_j \subseteq \mathcal{T}_j, \forall j$.*
- (iii) *$\lim_{j \rightarrow \infty} \mathcal{T}_j \equiv \bigcap_j \mathcal{T}_j \subseteq \mathcal{R}$.*

Proof. The proof of the first two statements is straightforward. Convergence is proven via contradiction along the following line: first, one uses the result given in [29] to provide a necessary and sufficient criterion for two qubit entanglement in terms of the renormalized expectation values. Alternatively one can also employ the criterion from [30]. Second, one derives a necessary condition for non-negativity of the reduced expectation value map τ_j in the limit $j \rightarrow \infty$, expressed again in terms of the renormalized expectation values of the spin-1 state. The two given conditions are mutually exclusive, hence no entangled state can be part of the superset \mathcal{T}_j in the limit $j \rightarrow \infty$. This shows convergence to the separable states in the end, since separable spin-1 states are trivially part of the outer approximation.

For a given direction $\hat{n} \in \mathbb{R}^3$ the corresponding spin operator in this direction is defined by $\mathcal{L}_{\hat{n}}^{(j)} = \partial\pi_j(\hat{n} \cdot \vec{\sigma}/2)$, and $\vec{\sigma}$ denotes the vector of Pauli matrices. Let $u_{\hat{n}}$ and $v_{\hat{n}}$ denote the corresponding renormalized expectation values of this spin operator given by equation (13). Using the result given in [29], the reduced two-qubit state ρ_j only supported on the symmetric subspace is entangled iff there exists a direction \hat{n} , such that $v_{\hat{n}} - u_{\hat{n}}^2 < 0$ holds.

The reduced expectation value matrix of order j of a given spin-1 density operator ρ , $\tau_j(\rho)$ is positive semidefinite iff all principle minors are non-negative. Using the unitary freedom of the matrix representation, in combination with the non-negativity of all possible 2×2 submatrices ensures that $\text{Var}(\mathcal{L}_{\hat{n}}^{(j)})/j^2 \geq 0$ for all possible directions \hat{n} . If one re-expresses this condition in the normalized expectation values one arrives at

$$v_{\hat{n}} - u_{\hat{n}}^2 + \frac{1}{2j}(1 - v_{\hat{n}}) \geq 0, \quad (18)$$

which becomes $v_{\hat{n}} - u_{\hat{n}}^2 \geq 0$ in the limit $j \rightarrow \infty$. This condition ensures that the entanglement condition can never be met in the limit, and this proves the convergence. \square

5. Hyperplane characterization

In this part we discuss some general features of compatibility problems, in which one asks whether a certain set of expectation values are consistent with an operator set, similar to problem 1.1. Consider a set of linear operators on a finite-dimensional Hilbert space. Without loss of generality, only a set of linear independent, Hermitian operators need to be considered, because any operator can be decomposed into Hermitian operators, and linear dependencies in the operator set demand only trivial conditions on the corresponding expectation values.

Problem 5.1 (consistency problem). *Consider the set of linearly independent, Hermitian operators acting on a finite-dimensional Hilbert space \mathcal{H} , $\{A_i\}$ with $i = 1, \dots, n$. Given an expectation value vector $\mathbf{b} \in \mathbb{R}^n$, under which conditions do these expectation values originate from a quantum-mechanical state, i.e., $\exists \rho \in \mathcal{D}(\mathcal{H})$ such that $\text{tr}(A_i \rho) = b_i, \forall i$?*

Since the set of density operators $\mathcal{D}(\mathcal{H})$ is compact, and because of linearity of the map $\mathcal{M} : \mathcal{D}(\mathcal{H}) \rightarrow \mathbb{R}^n$ that assigns the corresponding expectation values to a given state, $\rho \mapsto \mathcal{M}(\rho)_i = \text{tr}(A_i \rho)$, the set of valid expectation values is also compact. According to the Hahn–Banach theorem, every expectation value vector outside this set can be separated by a corresponding hyperplane, in analogy to entanglement witnesses [26] for the separability problem. The following theorem summarizes the necessary properties of those hyperplanes and therefore provides a possible characterization of the set of quantum-mechanical expectation values. Given a particular expectation value vector, the search for the optimal hyperplane can be cast in the form of a semidefinite program [31], which can be solved efficiently with interior-point methods. The given proof is based on this idea and employs well-known duality relations from semidefinite programming, cf [31].

In the case of the considered $\mathfrak{su}(2)$ moment problem, a formulation in terms of a semidefinite program offers an efficient way to characterize the set of possible expectation values for low total spin numbers j , i.e., in situations where the approximation method fails to provide a good description. Note that if one uses the particular representation of the considered spin operators, then one recovers the characterization of Bose-extendible states in terms of witness operators similar as described in [20].

Theorem 5.1 (hyperplane characterization). *Given a set of linearly independent operators $\{A_i\}$ and an expectation value vector $\mathbf{b} \in \mathbb{R}^n$, it holds:*

- *The vector \mathbf{b} is non-quantum mechanical, if and only if there exists a hyperplane, characterized by the normal vector $z \in \mathbb{R}^n : Z = \sum z_i A_i \geq 0, \text{tr}(Z) = 1$, which detects it $z^T \mathbf{b} < 0$.*
- *The vector \mathbf{b} is quantum mechanical, if and only if for all hyperplanes, characterized by the normal vector $z \in \mathbb{R}^n : Z = \sum z_i A_i \geq 0, \text{tr}(Z) = 1$ it holds that $z^T \mathbf{b} \geq 0$.*

Proof. The Gram–Schmidt orthogonalization allows us to transform any set of arbitrary linear independent, Hermitian operators $\{A_i\}$ to an orthonormal set of Hermitian operators $\{S_i\}$, i.e., the operators satisfy $\text{tr}(S_i S_j) = \delta_{ij}$ and $\text{tr}(S_i) \propto \delta_{i1}$. The connection is one-to-one and the corresponding expectation value vector \mathbf{b} has to be transformed in the same way, which results in the new expectation value vector \mathbf{t} .

The set $\{S_i\}$ for $i = 1, \dots, n$ can be extended to a Hermitian operator basis $\{S_i\}$ with $i = 1, \dots, d^2$ and $d = \dim(\mathcal{H})$. This basis set $\{S_i\}$ satisfies again $\text{tr}(S_i S_j) = \delta_{ij}$ and $\text{tr}(S_i) \propto \delta_{i1}$, which states that the first operator is proportional to the identity, $S_1 = \mathbb{1}/\sqrt{d}$, and all other elements S_j for $j > 1$ are tracefree. Therefore every density operator can be expressed as $\rho = \sum_i x_i S_i$ with $x_i = \text{tr}(S_i \rho)$. It must hold $x_i = t_i$ for $i = 1, \dots, n$ since otherwise, the expectation values do not match. The remaining open parameters $x_i, \forall i = n+1, \dots, d^2$ must be chosen such that $\rho(\mathbf{x}) = \rho_{\text{fix}} + \rho_{\text{open}}(\mathbf{x}) \geq 0$ forms a positive semidefinite operator and we have defined the fixed part $\rho_{\text{fix}} = \sum t_i S_i$ and open part $\rho_{\text{open}}(\mathbf{x}) = \sum x_i S_i$ of the density operator. This can be cast into the form of a semidefinite program [31], given by $\min_{(\mathbf{x}, t)}$ t subjected to $F(\mathbf{x}, t) = \rho(\mathbf{x}) + t \mathbb{1} \geq 0$, with solution (\mathbf{x}^*, t^*) . If $t^* > 0$, then there exists no parameters \mathbf{x} such that $\rho(\mathbf{x}) \geq 0$, since otherwise t^* is not optimal. On the other hand, if $t^* \leq 0$ then $\rho(\mathbf{x}^*) \geq 0$, and the expectation value vector \mathbf{t} is quantum mechanical.

Every semidefinite program has an associated dual program, cf [31], which reads $\max_Z (-\text{tr}(Z \rho_{\text{fix}}))$ subjected to $Z = \sum_{i=1}^n z_i S_i \geq 0$ and $\text{tr}(Z) = 1$. Using the orthogonality of the operators S_i , the objective value can be written as $\text{tr}(Z \rho_{\text{fix}}) = z^T \mathbf{t}$, and its optimal value is denoted by d^* . Note that both semidefinite programs are strictly feasible: if one selects $t > |\min \lambda(\rho_{\text{fix}})|$, where $\lambda(\cdot)$ denotes the corresponding eigenvalues, one obtains a strictly positive solution $F(\mathbf{x} = \mathbf{0}, t) > 0$ for the first program; the operator $Z = \mathbb{1}/d > 0$ provides a strictly positive solution for the second, dual program. These conditions ensure strong duality, which states equality of both programs $t^* = d^*$, and complementary slackness, which guarantees that there exist actual parameter sets for $(\mathbf{x}_{\text{opt}}, t_{\text{opt}})$, and Z_{opt} that attain the solutions t^* and d^* respectively, cf [31]. Therefore if \mathbf{t} is not quantum mechanical it holds that

$$-t^* = -d^* = \text{tr}(Z_{\text{opt}} \rho_{\text{fix}}) = z_{\text{opt}}^T \mathbf{t} < 0. \tag{19}$$

Hence every non-quantum-mechanical expectation value vector is detected by the corresponding hyperplane. In contrast, if \mathbf{t} is quantum mechanical, the weak duality condition [31] ensures that for every feasible solution z of the second program one has

$$z^T \mathbf{t} = \text{tr}(Z \rho_{\text{fix}}) \geq -t^* \geq 0, \tag{20}$$

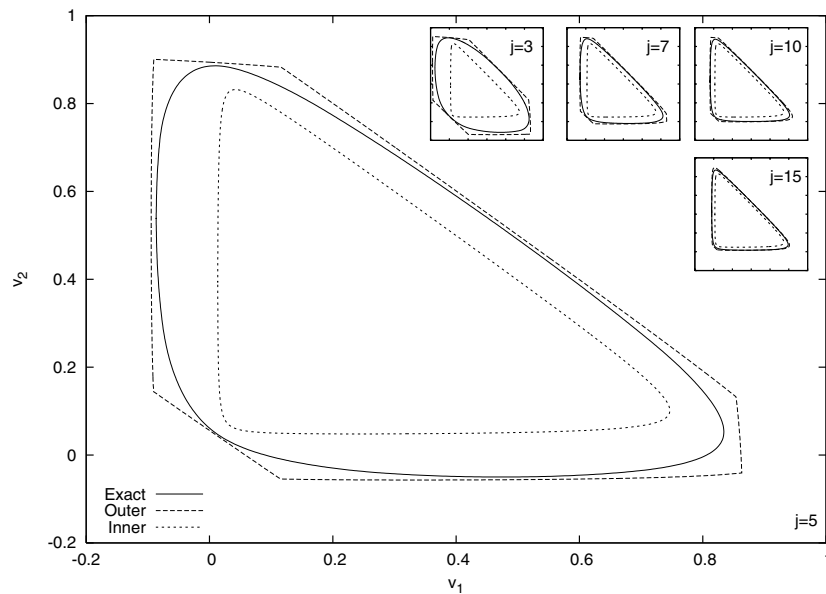


Figure 1. Sets of renormalized expectation values v_1 and v_2 described by the approximation in comparison with the exact solution for the case of $\vec{u} = (0.1, 0.2, 0.3)$. The inset figures are drawn with the same axis scale, and should demonstrate the effect of different total spin numbers j on the different sets.

so no quantum-mechanical expectation value vector is detected by the hyperplane. Using the described one-to-one correspondence allows us to translate these conditions back to the original operator set $\{A_i\}$, which delivers the result. \square

6. Visualization

The sets of renormalized expectation values that are determined by the described sub- and superset approximations enclose the set of quantum-mechanical expectation values, and convergence is reached in the case of infinite spin numbers j . In order to visualize each convex sets, one starts with given expectation values $u_k, k \in \{1, 2, 3\}$, which fulfill the condition $\sum_k u_k^2 \leq 1$, which ensures the existence of a quantum state, cf proposition 3.3. Next, the remaining open parameters v_k must be chosen according to the conditions from either an approximation set or from the exact solution. Using the Casimir identity, given by equation (2), allows us to further reduce the number of considered parameters v_k , and we choose v_1 and v_2 in the following. For both approximations, the search for the extremal values of the parameters v_k can be cast into the form of a semidefinite program, which can be efficiently solved by standard semidefinite program modules [32, 33]; for the exact solutions one needs to employ a semidefinite program anyway, cf section 5. Figure 1 shows the exact and the approximation sets for the case of $\vec{u} = (0.1, 0.2, 0.3)$ and total spin number $j = 5$. The inset figures visualize the same sets for different spin numbers j , and should demonstrate the corresponding convergence. The superset approximation seems to describe the actual set of quantum-mechanical expectation values with increasing accuracy as the total spin number j becomes larger.

7. Conclusion

We have addressed the problem whether a given set of expectation values can be compatible with the expectation values for products of two spin operators. Those operators, as abstractly introduced as the irreducible representations of an underlying $\mathfrak{su}(2)$ Lie algebra, appear for example as the Stokes operators in the quantum optics literature or as the total angular momentum operators in the case of atomic ensembles. Because of the particular product structure one can already impose a strong conditions on the given set of expectation values, which is summarized in positive semidefiniteness of a corresponding expectation value matrix that ensures the Schrödinger–Robertson uncertainty principle. Exploiting a particular representation of the $\mathfrak{su}(2)$ Lie algebra, allows us to relate the problem 1.1 to the Bose-symmetric extension problem for qubits, hence the following solution to problem 1.1 is provided: suppose that a given set of expectation values M satisfies the linear equality imposed by the Casimir identity, one reconstructs a particular two qubit operator $\rho_j(M)$. This operator $\rho_j(M)$ must represent a valid two qubit density operator of a bipartite qubit system with at least $2j - 2$ Bose-symmetric extensions, otherwise the given expectation values M disagree with the predictions of quantum mechanics. Since an exact characterization of two qubit states with a definite number of extensions is cumbersome, we consider in particular the two extreme cases. In particular, for large spin numbers we have presented two different approximating sets. Whenever one finds a separable two qubit state $\rho_j(M)$, then the expectation values can be assured to be quantum mechanical. Contrary, if one finds non-positivity of a particular expectation value matrix $\tau_j(\rho_j(M)) \not\geq 0$ that depends on the total spin number j and the reconstructed two-qubit state $\rho_j(M)$, then the corresponding expectation values are incompatible with the spin operators. In combination, both tools allow an *approximate operational* description of the quantum-mechanical expectation values. In particular, the presented method gets better the larger the total spin number j becomes, and convergence is assured in the limit of infinite numbers of extensions. In order to provide a feasible solution for low spin numbers, we characterize the sets of physical expectation values, similar as in problem 1.1, via hyperplanes. The search for the optimal hyperplane can be cast into the form of a semidefinite program which can be solved efficiently.

It remains open whether one can find an operational characterization of Bose-symmetric extendible two qubit states. In addition, it might be interesting to further investigate whether similar ideas can be used if one considers different Lie groups; we leave this open for future discussions.

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