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Bloch vectors for qudits

Reinhold A Bertlmann and Philipp Krammer

Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria

E-mail: reinhold.bertlmann@univie.ac.at and philipp.krammer@univie.ac.at

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Abstract

We present three different matrix bases that can be used to decompose density matrices of d-dimensional quantum systems, so-called qudits: the *generalized Gell–Mann matrix basis*, the *polarization operator basis* and the *Weyl operator basis*. Such a decomposition can be identified with a vector—the Bloch vector, i.e. a generalization of the well-known qubit case—and is a convenient expression for comparison with measurable quantities and for explicit calculations avoiding the handling of large matrices. We present a new method to decompose density matrices via so-called standard matrices, consider the important case of an isotropic two-qudit state and decompose it according to each basis. In the case of qutrits we show a representation of an entanglement witness in terms of expectation values of spin-1 measurements, which is appropriate for an experimental realization.

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1. Introduction

The state of a d-dimensional quantum system—a qudit—is usually described by a $d \times d$ density matrix. For high dimensions, where the matrices become large (for composite systems of n particles the matrices are of even much larger dimension $d^n \times d^n$), a simple way to express density matrices is of great interest.

Since the space of matrices is a vector space, there exist bases of matrices which can be used to decompose any matrix. For qubits such a basis contains the three Pauli matrices, accordingly, a density matrix can be expressed by a three-dimensional vector, the *Bloch vector*, and any such vector has to lie within the so-called *Bloch ball* [1, 2]. Unique for qubits is the fact that any point on the sphere, *Bloch sphere*, and inside the ball corresponds to a physical state, i.e. a density matrix. The pure states lie on the sphere and the mixed ones inside.

In higher dimensions there exist different matrix bases that can be used to express qudits as $(d^2 - 1)$-dimensional vectors as well. Different to the qubit case, however, is that the map induced is not bijective: not every point on the 'Bloch sphere' in dimensions $d^2 - 1$

corresponds to a physical state. Nevertheless the vectors are often also called 'Bloch vectors' (see in this context, e.g., [3–7]).

In this paper we want to present and compare three different matrix bases for a Bloch vector decomposition of qudits. In section 2 we propose the properties of any matrix basis for using it as a 'practical' decomposition of density matrices and recall the general notation of Bloch vectors. In sections 3–5 we offer three different matrix bases: the *generalized Gell–Mann matrix basis*, the *polarization operator basis* and the *Weyl operator basis*. For all these bases we give examples in the dimensions of our interest and present the different Bloch vector decompositions of an arbitrary density matrix in the standard matrix notation. Next in section 6, by constructing tensor products of states we study the isotropic two-qudit state and present the results for the three matrix decompositions, i.e. for the three different Bloch vectors. In section 7 we focus on the isotropic two-qudit state and calculate the Hilbert–Schmidt measure of entanglement (see, e.g., [8–11]). Its connection to the optimal entanglement witness is shown, which is determined in terms of the three matrix bases. An example for the experimental realization of an entanglement witness is given in section 7.2. The mathematical and physical advantages/disadvantages by using the three different matrix bases are discussed in section 8, where the final conclusions are also drawn.

2. Preliminaries

A *qudit* state is represented by a density operator in the Hilbert–Schmidt space acting on the d-dimensional Hilbert space $\mathcal{H}^d$ that can be written as a matrix—the density matrix—in the *standard basis* $\{|k\rangle\}$, with $k = 1, 2, \ldots, d$ or $k = 0, 1, 2, \ldots, d-1$.

Properties of a 'practical' matrix basis. For practical reasons the general properties of a matrix basis which is used for the Bloch vector decomposition of qudits are the following:

(i) The basis includes the identity matrix $\mathbb{1}$ and $d-1$ matrices $\{A_i\}$ of dimension $d \times d$ which are traceless, i.e. $\mathrm{Tr}\, A_i = 0$.
(ii) The matrices of any basis $\{A_i\}$ are orthogonal, i.e.

$$\mathrm{Tr}\, A_i^\dagger A_j = N\delta_{ij} \qquad \text{with} \quad N \in \mathbb{R}. \tag{1}$$

Bloch vector expansion of a density matrix. Since any matrix in the Hilbert–Schmidt space of dimension d can be decomposed with a matrix basis $\{A_i\}$, we can of course decompose a qudit density matrix as well and get the *Bloch vector expansion* of the density matrix,

$$\rho = \frac{1}{d}\mathbb{1} + \vec{b}\cdot\vec{\Gamma}, \tag{2}$$

where $\vec{b}\cdot\vec{\Gamma}$ is a linear combination of all matrices $\{A_i\}$ and the vector $\vec{b} \in \mathbb{R}^{d^2-1}$ with $b_i = \langle\Gamma_i\rangle = \mathrm{Tr}\,\rho\Gamma_i$ is called *Bloch vector*. The term $\frac{1}{d}\mathbb{1}$ is fixed because of condition $\mathrm{Tr}\,\rho = 1$.

Remark. Note that a given density matrix ρ can always be decomposed into a Bloch vector, but not any vector σ that is of form (2) is automatically a density matrix, even if it satisfies the conditions $\mathrm{Tr}\,\sigma = 1$ and $\mathrm{Tr}\,\sigma^2 \leqslant 1$ since generally it does not imply $\sigma \geqslant 0$.

Each different matrix basis induces a different Bloch vector lying within a Bloch hypersphere where, however, not every point of the hypersphere corresponds to a physical state (with $\rho \geqslant 0$); these points are excluded (holes). The geometric character of the Bloch space in higher dimensions turns out to be quite complicated and is still of great interest (see [3–7]).

All different Bloch hyperballs are isomorphic since they correspond to the same density matrix ρ. The interesting question is which Bloch hyperball—which matrix basis—is optimal for a specific purpose, such as the calculation of the entanglement degree or the determination of the geometry of the Hilbert space or the comparison with measurable quantities.

3. The generalized Gell–Mann matrix basis

3.1. Definition and example

The generalized Gell–Mann matrices (GGM) are higher-dimensional extensions of the Pauli matrices (for qubits) and the Gell–Mann matrices (for qutrits), they are the standard SU(N) generators (in our case $N = d$). They are defined as three different types of matrices and for simplicity we use here the operator notation, then the density matrices follow by simply writing the operators in the standard basis (see, e.g. [3, 12]):

(i) $\frac{d(d-1)}{2}$ symmetric GGM

$$\Lambda_s^{jk} = |j\rangle\langle k| + |k\rangle\langle j|, \qquad 1 \leqslant j < k \leqslant d; \tag{3}$$

(ii) $\frac{d(d-1)}{2}$ antisymmetric GGM

$$\Lambda_a^{jk} = -\mathrm{i}|j\rangle\langle k| + \mathrm{i}|k\rangle\langle j|, \qquad 1 \leqslant j < k \leqslant d; \tag{4}$$

(iii) $(d-1)$ diagonal GGM

$$\Lambda^l = \sqrt{\frac{2}{l(l+1)}}\left(\sum_{j=1}^{l}|j\rangle\langle j| - l|l+1\rangle\langle l+1|\right), \qquad 1 \leqslant l \leqslant d-1. \tag{5}$$

In total we have $d^2 - 1$ GGM; it follows from the definitions that all GGM are Hermitian and traceless. They are orthogonal and form a basis, the generalized Gell–Mann matrix basis (GGB). A proof for the orthogonality of GGB we present in appendix A.1.

Examples. Let us recall the case of dimension 3, the eight Gell–Mann matrices (for a representation see, e.g., [11, 13])

(i) three symmetric Gell–Mann matrices

$$\lambda_s^{12} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_s^{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \lambda_s^{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \tag{6}$$

(ii) three antisymmetric Gell–Mann matrices

$$\lambda_a^{12} = \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_a^{13} = \begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix}, \qquad \lambda_a^{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}; \tag{7}$$

(iii) two diagonal Gell–Mann matrices

$$\lambda^1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \lambda^2 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \tag{8}$$

To see how they generalize for higher dimensions we show the case we need for qudits of dimension $d = 4$:

(i) six symmetric GGM

$$\Lambda_s^{12} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_s^{13} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_s^{14} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$
$$\Lambda_s^{23} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_s^{24} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \Lambda_s^{34} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}; \tag{9}$$

(ii) six antisymmetric GGM

$$\Lambda_a^{12} = \begin{pmatrix} 0 & -\mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_a^{13} = \begin{pmatrix} 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_a^{14} = \begin{pmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \end{pmatrix},$$
$$\Lambda_a^{23} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_a^{24} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 0 \end{pmatrix}, \quad \Lambda_a^{34} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & \mathrm{i} & 0 \end{pmatrix}; \tag{10}$$

(iii) three diagonal GGM

$$\Lambda^1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda^2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda^3 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}. \tag{11}$$

Using the GGB we obtain, in general, the following Bloch vector expansion of a density matrix:

$$\rho = \frac{1}{d}\mathbb{1} + \vec{b} \cdot \vec{\Lambda}, \tag{12}$$

with the Bloch vector $\vec{b} = \left(\left\{b_s^{jk}\right\}, \left\{b_a^{jk}\right\}, \{b^l\}\right)$, where the components are ordered and for the indices we have the restrictions $1 \leqslant j < k \leqslant d$ and $1 \leqslant l \leqslant d-1$. The components are given by $b_s^{jk} = \mathrm{Tr}\,\Lambda_s^{jk}\rho$, $b_a^{jk} = \mathrm{Tr}\,\Lambda_a^{jk}\rho$ and $b^l = \mathrm{Tr}\,\Lambda^l\rho$. All Bloch vectors lie within a hypersphere of radius $|\vec{b}| \leqslant \sqrt{(d-1)/2d}$. For example, for qutrits the Bloch vector components are $\vec{b} = \left(b_s^{12}, b_s^{13}, b_s^{23}, b_a^{12}, b_a^{13}, b_a^{23}, b^1, b^2\right)$ corresponding to the Gell–Mann matrices (6)–(8) and $|\vec{b}| \leqslant \sqrt{1/3}$.

As already mentioned the allowed range of $\vec{b}$ is restricted. It has an interesting geometric structure which has been calculated analytically for the case of qutrits by studying two-dimensional planes in the eight-dimensional Bloch space [3] or numerically by considering three-dimensional cross-sections [7]. In any case, pure states lie on the surface and the mixed ones inside.

3.2. Standard matrix basis expansion by GGB

The standard matrices are simply the $d \times d$ matrices that have only one entry 1 and the other entries 0 and form an orthonormal basis of the Hilbert–Schmidt space. We write these matrices shortly as operators

$$|j\rangle\langle k|, \qquad \text{with} \quad j, k = 1, \ldots, d. \tag{13}$$

Any matrix can easily be decomposed into a 'vector' via a certain linear combination of matrices (13). Knowing the expansion of matrices (13) into GGB we can therefore find the decomposition of any matrix in terms of the GGB.

We find the following expansion of standard matrices (13) into GGB :

$$|j\rangle\langle k| = \begin{cases} \frac{1}{2}\left(\Lambda_s^{jk} + \mathrm{i}\Lambda_a^{jk}\right) & \text{for} \quad j < k \\ \frac{1}{2}\left(\Lambda_s^{kj} - \mathrm{i}\Lambda_a^{kj}\right) & \text{for} \quad j > k \\ -\sqrt{\frac{j-1}{2j}}\Lambda^{j-1} + \sum_{n=0}^{d-j-1} \frac{1}{\sqrt{2(j+n)(j+n+1)}}\Lambda^{j+n} + \frac{1}{d}\mathbb{1} & \text{for} \quad j = k. \end{cases} \tag{14}$$

Proof. The first two cases can be easily verified.

To show the last case we first set up a recurrence relation for $|l\rangle\langle l|$, which we obtain by eliminating the term $\sum_{j=1}^{l-1} |j\rangle\langle j|$ in the two expressions (5) for Λ^l and Λ^{l-1}

$$|l\rangle\langle l| = -\sqrt{\frac{l-1}{2l}}\Lambda^{l-1} + \sqrt{\frac{l+1}{2l}}\Lambda^l + |l+1\rangle\langle l+1|, \tag{15}$$

and we consider the case $l + 1 = d$

$$|d-1\rangle\langle d-1| = -\sqrt{\frac{d-2}{2(d-1)}}\Lambda^{d-2} + \sqrt{\frac{d}{2(d-1)}}\Lambda^{d-1} + |d\rangle\langle d|. \tag{16}$$

From Λ^{d-1} given by equation (5)

$$\Lambda^{d-1} = \sqrt{\frac{2}{(d-1)d}}\left(\sum_{j=1}^{d-1} |j\rangle\langle j| - (d-1)|d\rangle\langle d|\right), \tag{17}$$

we get the Bloch vector decomposition of $|d\rangle\langle d|$

$$|d\rangle\langle d| = \frac{1}{d}\left(-\sqrt{\frac{(d-1)d}{2}}\Lambda^{d-1} + \mathbb{1}\right), \tag{18}$$

where we have applied $\sum_{j=1}^{d-1} |j\rangle\langle j| = \mathbb{1} - |d\rangle\langle d|$.

Inserting now decomposition (18) into relation (16) we gain the Bloch vector expansion for $|d-1\rangle\langle d-1|$ and recurrence relation (15) provides $|d-2\rangle\langle d-2|$ and so forth. Thus finally we find

$$|d-n\rangle\langle d-n| = -\sqrt{\frac{d-n-1}{2(d-n)}}\Lambda^{d-n-1} + \sum_{k=0}^{n-1} \frac{1}{\sqrt{2(d-n+k+1)(d-n+k)}}\Lambda^{d-n+k} + \frac{1}{d}\mathbb{1}, \tag{19}$$

the relation we had to prove, where $d - n = j$. □

4. The polarization operator basis

4.1. Definition and examples

The polarization operators in the Hilbert–Schmidt space of dimension d are defined as the following $d \times d$ matrices [4, 14] :

$$T_{LM} = \sqrt{\frac{2L+1}{2s+1}} \sum_{k,l=1}^{d} C^{sm_k}_{sm_l,LM} |k\rangle\langle l|. \tag{20}$$

The used indices have the properties

$$\begin{aligned} &s = \frac{d-1}{2}, \\ &L = 0, 1, \ldots, 2s, \\ &M = -L, -L+1, \ldots, L-1, L, \\ &m_1 = s, m_2 = s-1, \ldots, m_d = -s. \end{aligned} \tag{21}$$

The coefficients $C^{sm_k}_{sm_l,LM}$ are identified with the usual Clebsch–Gordan coefficients $C^{jm}_{j_1m_1,j_2m_2}$ of the angular momentum theory and are displayed explicitly in tables, e.g., in [14].

For $L = M = 0$ the polarization operator is proportional to the identity matrix [4, 14],

$$T_{00} = \frac{1}{\sqrt{d}} \mathbb{1}. \tag{22}$$

It is shown in [4] that all polarization operators (except T_{00}) are traceless, in general *not* Hermitian, and that orthogonality relation (1) is satisfied

$$\mathrm{Tr}\, T^{\dagger}_{L_1M_1} T_{L_2M_2} = \delta_{L_1L_2} \delta_{M_1M_2}. \tag{23}$$

Therefore the d^2 polarization operators (20) form an orthonormal matrix basis—the polarization operator basis (POB)—of the Hilbert–Schmidt space of dimension d.

Examples. The simplest example is of dimension 2, the qubit. For a qubit the POB is given by the following matrices ($s = 1/2$; $L = 0, 1$; $M = -1, 0, 1$):

$$\begin{aligned} T_{00} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad T_{11} = -\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \\ T_{10} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad T_{1-1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \end{aligned} \tag{24}$$

For the next higher dimension $d = 3$ ($s = 1$), the case of qutrits, we get nine polarization operators T_{LM} with $L = 0, 1, 2$ and $M = -L, \ldots, L$ and we have

$$\begin{aligned} &T_{11} = -\frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad T_{10} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad T_{1-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \\ &T_{22} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T_{21} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad T_{20} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\ &T_{2-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \quad T_{2-2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{25}$$

Then the decomposition of any density matrix into a Bloch vector by using the POB has, in general, the following form:

$$\rho = \frac{1}{d}\mathbb{1} + \sum_{L=1}^{2s}\sum_{M=-L}^{L} b_{LM}T_{LM} = \frac{1}{d}\mathbb{1} + \vec{b}\cdot\vec{T}, \tag{26}$$

with the Bloch vector $\vec{b} = (b_{1-1}, b_{10}, b_{11}, b_{2-2}, b_{2-1}, b_{20}, \ldots, b_{LM})$, where the components are ordered and given by $b_{LM} = \mathrm{Tr}\, T_{LM}^{\dagger}\rho$. In general the components b_{LM} are complex since the polarization operators T_{LM} are not Hermitian. All Bloch vectors lie within a hypersphere of radius $|\vec{b}| \leqslant \sqrt{(d-1)/d}$.

In two dimensions the Bloch vector $\vec{b} = (b_{1-1}, b_{10}, b_{11})$ is limited by $|\vec{b}| \leqslant \frac{1}{\sqrt{2}}$ and forms a spheroid [4], the pure states occupy the surface and the mixed ones lie in the volume. This decomposition is fully equivalent to the standard description of Bloch vectors with Pauli matrices.

In higher dimensions, however, the structure of the allowed range of $\vec{b}$ (due to the positivity requirement $\rho \geqslant 0$) is quite complicated, as can be seen already for $d = 3$ (for details, see [4]). Nevertheless, pure states are on the surface, mixed ones lie within the volume and the maximal mixed one corresponds to $|\vec{b}| = 0$, thus $|\vec{b}|$ is a kind of measure for the mixedness of a quantum state.

4.2. Standard matrix basis expansion by POB

The standard matrices (13) can be expanded by the POB as [14]

$$|i\rangle\langle j| = \sum_L\sum_M \sqrt{\frac{2L+1}{2s+1}}\, C^{sm_i}_{sm_j,LM} T_{LM}. \tag{27}$$

Note that $\sum_M$ is actually fixed by the condition $m_j + M = m_i$.

Proof. Inserting definition (20) on the right-hand side (RHS) of equation (27) we find

$$\begin{aligned} \mathrm{RHS} &= \sum_{k,l}\left(\sum_L \frac{2L+1}{2s+1} C^{sm_i}_{sm_j,LM} C^{sm_k}_{sm_l,LM}\right)|k\rangle\langle l| \\ &= \sum_{k,l}\delta_{jl}\delta_{ik}|k\rangle\langle l| \\ &= |i\rangle\langle j|, \end{aligned} \tag{28}$$

where we used the sum rule for Clebsch–Gordan coefficients [14]

$$\sum_{c,\gamma}\frac{2c+1}{2b+1} C^{b\beta}_{a\alpha,c\gamma} C^{b\beta'}_{a\alpha',c\gamma} = \delta_{\alpha\alpha'}\delta_{\beta\beta'}. \tag{29}$$

□

5. Weyl operator basis

5.1. Definition and example

Finally, we want to discuss a basis of the Hilbert–Schmidt space of dimension d that consists of the following d^2 operators:

$$U_{nm} = \sum_{k=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}kn}|k\rangle\langle (k+m)\,\mathrm{mod}\, d| \qquad n, m = 0, 1, \ldots, d-1, \tag{30}$$

where we use the standard basis of the Hilbert space.

The operators in notation (30) have been introduced in the context of quantum teleportation of qudit states [15] and are often called *Weyl operators* in the literature (see e.g. [16–18]). The d^2 operators (30) are unitary and form an orthonormal basis of the Hilbert–Schmidt space

$$\mathrm{Tr}\, U_{nm}^{\dagger} U_{lj} = d\delta_{nl}\delta_{mj} \tag{31}$$

(a proof is presented in appendix A.3)—the Weyl operator basis (WOB). They can be used to create a basis of d^2 maximally entangled qudit states [16, 19, 20].

Clearly the operator U_{00} represents the identity $U_{00} = \mathbb{1}$.

Example. Let us show the example of dimension 3, the qutrit case. There the Weyl operators (30) have the following matrix form:

$$U_{01} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad U_{02} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$U_{10} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathrm{e}^{2\pi\mathrm{i}/3} & 0 \\ 0 & 0 & \mathrm{e}^{-2\pi\mathrm{i}/3} \end{pmatrix}, \quad U_{11} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \mathrm{e}^{2\pi\mathrm{i}/3} \\ \mathrm{e}^{-2\pi\mathrm{i}/3} & 0 & 0 \end{pmatrix}, \quad U_{12} = \begin{pmatrix} 0 & 0 & 1 \\ \mathrm{e}^{2\pi\mathrm{i}/3} & 0 & 0 \\ 0 & \mathrm{e}^{-2\pi\mathrm{i}/3} & 0 \end{pmatrix},$$

$$U_{20} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathrm{e}^{-2\pi\mathrm{i}/3} & 0 \\ 0 & 0 & \mathrm{e}^{2\pi\mathrm{i}/3} \end{pmatrix}, \quad U_{21} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \mathrm{e}^{-2\pi\mathrm{i}/3} \\ \mathrm{e}^{2\pi\mathrm{i}/3} & 0 & 0 \end{pmatrix}, \quad U_{22} = \begin{pmatrix} 0 & 0 & 1 \\ \mathrm{e}^{-2\pi\mathrm{i}/3} & 0 & 0 \\ 0 & \mathrm{e}^{2\pi\mathrm{i}/3} & 0 \end{pmatrix}. \tag{32}$$

Using the WOB we can decompose quite generally any density matrix into a Bloch vector

$$\rho = \frac{1}{d}\mathbb{1} + \sum_{n,m=0}^{d-1} b_{nm} U_{nm} = \frac{1}{d}\mathbb{1} + \vec{b}\cdot\vec{U}, \tag{33}$$

with $n, m = 0, 1, \ldots, d-1$ ($b_{00} = 0$). The components of the Bloch vector $\vec{b} = (\{b_{nm}\})$ are ordered and given by $b_{nm} = \mathrm{Tr}\, U_{nm}\rho$. In general the components b_{nm} are complex since the Weyl operators are not Hermitian and the complex conjugates fulfil the relation $b_{nm}^{*} = \mathrm{e}^{-\frac{2\pi\mathrm{i}}{d}nm} b_{-n-m}$, which follows easily from definition (30) together with the hermiticity of ρ.

All Bloch vectors lie within a hypersphere of radius $|\vec{b}| \leqslant \sqrt{d-1}/d$. For example, for qutrits the Bloch vector is expressed by $\vec{b} = (b_{01}, b_{02}, b_{10}, b_{11}, b_{12}, b_{20}, b_{21}, b_{22})$ and $|\vec{b}| \leqslant \sqrt{2}/3$. In three and higher dimensions the allowed range of the Bloch vector is quite restricted within the hypersphere and the detailed structure is not known yet.

Note that in two dimensions the WOB as well as the GGB coincides with the Pauli matrix basis and the POB represents a rotated Pauli basis (where $\sigma_{\pm} = \frac{1}{2}(\sigma_1 \pm \mathrm{i}\sigma_2)$), in particular

$$\{U_{00}, U_{01}, U_{10}, U_{11}\} = \{\mathbb{1}, \sigma_1, \sigma_3, \mathrm{i}\sigma_2\}, \tag{34}$$

$$\left\{\mathbb{1}, \lambda_s^{12}, \lambda_a^{12}, \lambda^1\right\} = \{\mathbb{1}, \sigma_1, \sigma_2, \sigma_3\}, \tag{35}$$

$$\{T_{00}, T_{11}, T_{10}, T_{1-1}\} = \left\{\tfrac{1}{\sqrt{2}}\mathbb{1}, -\sigma_+, \tfrac{1}{\sqrt{2}}\sigma_3, \sigma_-\right\}. \tag{36}$$

5.2. Standard matrix basis expansion by WOB

The standard matrices (13) can be expressed by the WOB in the following way:

$$|j\rangle\langle k| = \frac{1}{d}\sum_{l=0}^{d-1} \mathrm{e}^{-\frac{2\pi\mathrm{i}}{d}lj} U_{l(k-j)\mathrm{mod}\,d}. \tag{37}$$

Proof. We insert the definition of the Weyl operators (30) on the right-hand side of equation (37), use equation (A.24) and get

$$\begin{aligned} \text{RHS} &= \frac{1}{d}\sum_{l,r=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} l(r-j)} |r\rangle\langle (r+k-j) \bmod d| \\ &= |j\rangle\langle k| + \frac{1}{d}\sum_{r\neq j, r=0}^{d-1}\sum_{l=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} l(r-j)} |r\rangle\langle (r+k-j) \bmod d| \\ &= |j\rangle\langle k|. \end{aligned} \tag{38}$$

□

6. Isotropic two-qudit state

Now we consider bipartite systems in a $d \times d$-dimensional Hilbert space $\mathcal{H}_A^d \otimes \mathcal{H}_B^d$. The observables acting in the subsystems $\mathcal{H}_A$ and $\mathcal{H}_B$ are usually called Alice and Bob in quantum communication.

Quite generally, a density matrix of a two-qudit state acting on $\mathcal{H}_A^d \otimes \mathcal{H}_B^d$ can be decomposed in the following way (neglecting the reference to A and B):

$$\rho = \frac{1}{d}\mathbb{1} \otimes \mathbb{1} + n_i \Gamma_i \otimes \mathbb{1} + m_i \mathbb{1} \otimes \Gamma_i + c_{ij}\Gamma_i \otimes \Gamma_j, \qquad n_i, m_i, c_{ij} \in \mathbb{C}, \tag{39}$$

where $\{\Gamma_i\}$ represents some basis in the subspace $\mathcal{H}^d$. The term $c_{ij}\Gamma_i \otimes \Gamma_j$ always can be diagonalized by two independent orthogonal transformations on Γ_i and Γ_j [21]. Altogether there are $(d^2)^2 - 1$ terms.

However, for isotropic two-qudit states—the case we consider in our paper—the second and third terms in expression (39) vanish and the fourth term reduces to $c_{ii}\Gamma_i \otimes \Gamma_i$, which implies the vanishing of $(d^2-1)^2 + (d^2-1) = d^2(d^2-1)$ terms. Consequently, for an isotropic two-qudit density matrix there remain $d^2 - 1$ independent terms, which provides the dimension of the corresponding Bloch vector. Thus the isotropic two-qudit Bloch vector is of the same dimension—lives in the same subspace—as the one-qudit vector, which is a comfortable simplification.

Explicitly, the *isotropic* two-qudit state $\rho_\alpha^{(d)}$ is defined as follows [22–24]:

$$\rho_\alpha^{(d)} = \alpha \left|\phi_+^d\right\rangle\left\langle\phi_+^d\right| + \frac{1-\alpha}{d^2}\mathbb{1}, \qquad \alpha \in \mathbb{R}, \qquad -\frac{1}{d^2-1} \leqslant \alpha \leqslant 1, \tag{40}$$

where the range of α is determined by the positivity of the state. The state $\left|\phi_+^d\right\rangle$, a Bell state, is maximally entangled and given by

$$\left|\phi_+^d\right\rangle = \frac{1}{\sqrt{d}}\sum_j |j\rangle \otimes |j\rangle, \tag{41}$$

where $\{|j\rangle\}$ denotes the standard basis of the d-dimensional Hilbert space.

6.1. Expansion into GGB

Let us first calculate the Bloch vector notation for the Bell state $\left|\phi_+^d\right\rangle\left\langle\phi_+^d\right|$ in the GGB. It is convenient to split the state into two parts

$$\begin{aligned} \left|\phi_+^d\right\rangle\left\langle\phi_+^d\right| &= \frac{1}{d}\sum_{j,k=1}^{d} |j\rangle\langle k| \otimes |j\rangle\langle k| \\ &= A + B, \end{aligned} \tag{42}$$

where A and B are defined by

$$A := \frac{1}{d}\sum_{j<k} |j\rangle\langle k| \otimes |j\rangle\langle k| + \frac{1}{d}\sum_{j<k} |k\rangle\langle j| \otimes |k\rangle\langle j|, \tag{43}$$

$$B := \frac{1}{d}\sum_{j} |j\rangle\langle j| \otimes |j\rangle\langle j|, \tag{44}$$

and to calculate the two terms separately.

For term A we use the standard matrix expansion (14) for the case $j \neq k$ and get

$$\begin{aligned} A &= \frac{1}{4d}\left[\sum_{j<k}\left(\Lambda_s^{jk} + \mathrm{i}\Lambda_a^{jk}\right)\otimes\left(\Lambda_s^{jk} + i\Lambda_a^{jk}\right) + \sum_{j<k}\left(\Lambda_s^{jk} - \mathrm{i}\Lambda_a^{jk}\right)\otimes\left(\Lambda_s^{jk} - \mathrm{i}\Lambda_a^{jk}\right)\right] \\ &= \frac{1}{2d}\sum_{i<j}\left(\Lambda_s^{jk}\otimes\Lambda_s^{jk} - \Lambda_a^{jk}\otimes\Lambda_a^{jk}\right). \end{aligned} \tag{45}$$

For term B we need the case $j = k$ in expansion (14) and obtain after some calculations (the details are presented in appendix A.2)

$$B = \frac{1}{2d}\sum_{m=1}^{d-1} \Lambda^m \otimes \Lambda^m + \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1}. \tag{46}$$

Thus all together we find the following GGB Bloch vector notations, for the Bell state (42):

$$\left|\phi_+^d\right\rangle\left\langle\phi_+^d\right| = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{1}{2d}\Lambda, \tag{47}$$

and for the isotropic two-qudit state (40)

$$\rho_\alpha^{(d)} = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{\alpha}{2d}\Lambda, \tag{48}$$

where we defined

$$\Lambda := \sum_{i<j} \Lambda_s^{jk}\otimes\Lambda_s^{jk} - \sum_{i<j}\Lambda_a^{jk}\otimes\Lambda_a^{jk} + \sum_{m=1}^{d-1}\Lambda^m\otimes\Lambda^m. \tag{49}$$

6.2. Expansion into POB

Now we calculate the Bell state $\left|\phi_+^d\right\rangle\left\langle\phi_+^d\right|$ in the POB. Using expansion (27) and the sum rule for the Clebsch–Gordan coefficients [14]

$$\sum_{\alpha,\gamma} C^{c\gamma}_{a\alpha,b\beta} C^{c\gamma}_{a\alpha,b'\beta'} = \frac{2c+1}{2b+1}\delta_{bb'}\delta_{\beta\beta'}, \tag{50}$$

we obtain

$$\begin{aligned} \left|\phi_+^d\right\rangle\left\langle\phi_+^d\right| &= \frac{1}{d}\sum_{i,j=1}^{d} |i\rangle\langle j| \otimes |i\rangle\langle j| \\ &= \frac{1}{d}\sum_{L,L'} \frac{\sqrt{(2L+1)(2L'+1)}}{2s+1}\left(\sum_{i,j} C^{sm_i}_{sm_j,LM} C^{sm_i}_{sm_j,L'M}\right) T_{LM}\otimes T_{L'M} \\ &= \frac{1}{d}\sum_{L,L'} \frac{\sqrt{(2L+1)(2L'+1)}}{2L+1}\delta_{L,L'} T_{LM}\otimes T_{L'M} \end{aligned}$$

$$= \frac{1}{d}\sum_L T_{LM}\otimes T_{LM}$$

$$= \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{1}{d}T, \tag{51}$$

where we extracted the unity (recall equation (22)) and defined

$$T := \sum_{L,M\neq 0,0} T_{LM}\otimes T_{LM}. \tag{52}$$

Result (51) provides the POB Bloch vector notation of the isotropic two-qudit state (40)

$$\rho_\alpha^{(d)} = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{\alpha}{d}T. \tag{53}$$

6.3. Expansion into WOB

Finally, we present the Bell state in the WOB (the details for our approach using the standard matrix expression (37) can be found in appendix A.4, see also [16])

$$\left|\phi_+^d\right\rangle\left\langle\phi_+^d\right| = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{1}{d^2}U, \tag{54}$$

with

$$U := \sum_{l,m=0}^{d-1} U_{lm}\otimes U_{-lm}, \qquad (l,m)\neq(0,0), \tag{55}$$

where negative values of the index l have to be considered as mod d, and from formula (54) we find the WOB Bloch vector notation of the isotropic two-qudit state

$$\rho_\alpha^{(d)} = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{\alpha}{d^2}U. \tag{56}$$

7. Applications of the matrix bases

7.1. Entangled isotropic two-qudit states

In [11] the connection between the Hilbert–Schmidt (HS) measure of entanglement [8–10] and the optimal entanglement witness is investigated. Explicit calculations for both quantities are presented in the case of isotropic qutrit states. For higher dimensions, the isotropic two-qudit states, the above quantities are determined as well but in terms of a rather general matrix basis decomposition. With the results of the present paper we can calculate all quantities explicitly. Let us recall the basic notations we need.

The HS *measure* is defined as the minimal HS distance of an entangled state ρ_{ent} to the set of separable states S

$$D(\rho_{\text{ent}}) := \min_{\rho\in S}\|\rho-\rho_{\text{ent}}\| = \|\rho_0-\rho_{\text{ent}}\|, \tag{57}$$

where ρ_0 denotes the nearest separable state, the minimum of the HS distance.

An *entanglement witness* $A\in\mathcal{A}$ ($\mathcal{A}=\mathcal{A}_A\otimes\mathcal{A}_B$, the HS space of operators acting on the Hilbert space of states) is a Hermitian operator that 'detects' the entanglement of a state ρ_{ent} via inequalities [10, 25–27].

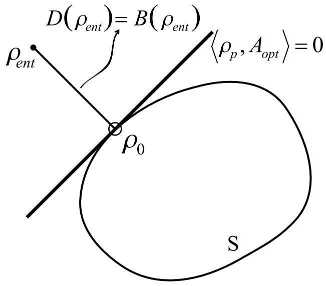

Figure 1. Illustration of the Bertlmann–Narnhofer–Thirring theorem (62).

Definition 1. *An entanglement witness A is an operator with the following properties: the expectation value of A is negative for an entangled state, whereas it is non-negative for any separable state.*

$$\begin{aligned} \langle \rho_{\text{ent}}, A \rangle &= \text{Tr}\, \rho_{\text{ent}} A < 0, \\ \langle \rho, A \rangle &= \text{Tr}\, \rho A \geqslant 0 \qquad \forall \rho \in S. \end{aligned} \tag{58}$$

The fact, however that there exists a Hermitian operator satisfying inequalities (58) for *any* entangled state, i.e. that the definition is meaningful, has to be proved; it follows from the Hahn–Banach theorem of functional analysis (for a simple geometric approach, see [11]).

An entanglement witness is 'optimal', denoted by A_{opt}, if apart from equation (58) there exists a separable state $\rho_0 \in S$ such that

$$\langle \rho_0, A_{\text{opt}} \rangle = 0. \tag{59}$$

The operator A_{opt} defines a tangent plane to the set of separable states S and all states ρ_p with $\langle \rho_p, A_{\text{opt}} \rangle = 0$ lie within that plane; see figure 1.

Let us call the lower one of the inequalities (58) an *entanglement witness inequality*, EWI. It detects entanglement whereas a Bell inequality determines non-locality. Rewriting equation (58) as

$$\langle \rho, A \rangle - \langle \rho_{\text{ent}}, A \rangle \geqslant 0 \qquad \forall \rho \in S, \tag{60}$$

the *maximal violation* of the EWI is defined by

$$B(\rho_{\text{ent}}) = \max_{A, \|A - a\mathbb{1}\| \leqslant 1} \left(\min_{\rho \in S} \langle \rho, A \rangle - \langle \rho_{\text{ent}}, A \rangle \right), \tag{61}$$

where the maximum is taken over all possible entanglement witnesses A, suitably normalized.

Then an interesting connection between the HS measure and the concept of entanglement witnesses is given by the Bertlmann–Narnhofer–Thirring theorem, illustrated in figure 1 [10].

Theorem 1.

(i) The maximal violation of the EWI is equal to the minimal distance of ρ_{ent} to the set S

$$B(\rho_{\text{ent}}) = D(\rho_{\text{ent}}). \tag{62}$$

(ii) The maximal violation of the EWI is attained for an optimal entanglement witness

$$A_{\text{opt}} = \frac{\rho_0 - \rho_{\text{ent}} - \langle \rho_0, \rho_0 - \rho_{\text{ent}} \rangle \mathbb{1}}{\|\rho_0 - \rho_{\text{ent}}\|}. \tag{63}$$

Thus the calculation of the optimal entanglement witness A_{opt} to a given entangled state ρ_{ent} reduces to the determination of the nearest separable state ρ_0. In special cases ρ_0 is detectable but in general its detection is quite a difficult task. We are able to find the nearest separable state by working with lemma 1, a method we call *guess method* [11].

Lemma 1. *A state $\tilde{\rho}$ is equal to the nearest separable state ρ_0 if and only if the operator*

$$\tilde{C} = \frac{\tilde{\rho} - \rho_{\mathrm{ent}} - \langle\tilde{\rho}, \tilde{\rho} - \rho_{\mathrm{ent}}\rangle \mathbb{1}}{\|\tilde{\rho} - \rho_{\mathrm{ent}}\|} \tag{64}$$

is an entanglement witness.

Lemma 1 probes if a guess $\tilde{\rho}$ is indeed correct for the nearest separable state, then operator $\tilde{C}$ represents the optimal entanglement witness A_{opt} (63).

Now let us apply the matrix bases we discussed in the previous sections and calculate the quantities introduced above. As an entangled state we consider the isotropic two-qudit state $\rho_\alpha^{(d),\mathrm{ent}}$, that is the state $\rho_\alpha^{(d)}$ (40) for $\frac{1}{d+1} < \alpha \leqslant 1$.

Starting with the GGB we can express that state in our Bloch vector notation by formula (48). By using lemma 1 we find that the nearest separable state is reached at $\alpha = \frac{1}{d+1}$

$$\rho_0^{(d)} = \rho_{\alpha=\frac{1}{d+1}}^{(d)} = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{1}{2d(d+1)}\Lambda. \tag{65}$$

It provides the HS measure

$$D\big(\rho_{\alpha,\mathrm{ent}}^{(d)}\big) = \big\|\rho_0^{(d)} - \rho_{\alpha,\mathrm{ent}}^{(d)}\big\| = \frac{\sqrt{d^2-1}}{d}\left(\alpha - \frac{1}{d+1}\right), \tag{66}$$

and the optimal entanglement witness (63)

$$A_{\mathrm{opt}}\big(\rho_{\alpha,\mathrm{ent}}^{(d)}\big) = \frac{1}{d}\sqrt{\frac{d-1}{d+1}}\mathbb{1}\otimes\mathbb{1} - \frac{1}{2\sqrt{d^2-1}}\Lambda, \tag{67}$$

where we used the HS norm $\|\Lambda\| = 2\sqrt{d^2-1}$.

Clearly, the maximal violation B of the EWI equals the HS measure D

$$\begin{aligned} B\big(\rho_{\alpha,\mathrm{ent}}^{(d)}\big) &= -\big\langle\rho_{\alpha,\mathrm{ent}}^{(d)}, A_{\mathrm{opt}}\big\rangle \\ &= \frac{\sqrt{d^2-1}}{d}\left(\alpha - \frac{1}{d+1}\right) = D\big(\rho_{\alpha,\mathrm{ent}}^{(d)}\big). \end{aligned} \tag{68}$$

For expressing above quantities by the matrix bases POB and WOB it suffices to calculate the proportionality factors between Λ, T and U. By comparison of the three forms for the isotropic qudit state (48), (53) and (56) we find

$$\Lambda = 2T \qquad \text{and} \qquad T = \frac{1}{d}U. \tag{69}$$

It provides the following expressions, for the POB

$$\rho_0^{(d)} = \rho_{\alpha=\frac{1}{d+1}}^{(d)} = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{1}{d(d+1)}T, \tag{70}$$

$$A_{\mathrm{opt}}(\rho_{\alpha,\mathrm{ent}}^{(d)}) = \frac{1}{d}\sqrt{\frac{d-1}{d+1}}\mathbb{1}\otimes\mathbb{1} - \frac{1}{\sqrt{d^2-1}}T, \tag{71}$$

and for the WOB

$$\rho_0^{(d)} = \rho^{(d)}_{\alpha=\frac{1}{d+1}} = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{1}{d^2(d+1)}U, \tag{72}$$

$$A_{\mathrm{opt}}\left(\rho^{(d)}_{\alpha,\mathrm{ent}}\right) = \frac{1}{d}\sqrt{\frac{d-1}{d+1}}\mathbb{1}\otimes\mathbb{1} - \frac{1}{d\sqrt{d^2-1}}U. \tag{73}$$

Of course, the HS measure $D\left(\rho^{(d)}_{\alpha,\mathrm{ent}}\right)$ remains the same expression (66) independent of the chosen matrix basis, which can easily be verified using $\|T\| = \sqrt{d^2-1}$ and $\|U\| = d\sqrt{d^2-1}$.

7.2. *Entanglement witness representation for experiments*

Entanglement witnesses are Hermitian operators and therefore observables that should be measurable in a given experimental set-up and thus provide an experimental verification of entanglement. The quantity to be measured is the expectation value

$$\langle A\rangle = \mathrm{Tr}\, A\rho \tag{74}$$

of an entanglement witness A for some state ρ. If $\langle A\rangle < 0$ then the state ρ is entangled. But which measurements have to be performed?

Obviously it is appropriate to express the entanglement witness in terms of generalized Gell–Mann matrices (3)–(5), since they are Hermitian. For $d = 3$—qutrits—the Gell–Mann matrices (6)–(8) can be expressed in terms of eight 'physical' operators, the observables $S_x, S_y, S_z, S_x^2, S_y^2, \{S_x, S_y\}, \{S_y, S_z\}, \{S_z, S_x\}$ of a spin-1 system, where $\vec{S} = (S_x, S_y, S_z)$ is the spin operator and $\{S_i, S_j\} = S_iS_j + S_jS_i$ (with $i, j = x, y, z$) denotes the corresponding anticommutator. The decomposition of the Gell–Mann matrices into spin-1 operators is as follows (for a similar expansion, see [7]):

$$\begin{aligned}
\lambda_s^{12} &= \frac{1}{\sqrt{2}\hbar^2}\left(\hbar S_x + \{S_z, S_x\}\right), & \lambda_s^{13} &= \frac{1}{\hbar^2}\left(S_x^2 - S_y^2\right), \\
\lambda_s^{23} &= \frac{1}{\sqrt{2}\hbar^2}\left(\hbar S_x - \{S_z, S_x\}\right), & \lambda_a^{12} &= \frac{1}{\sqrt{2}\hbar^2}(\hbar S_y + \{S_y, S_z\}), \\
\lambda_a^{13} &= \frac{1}{\hbar^2}\{S_x, S_y\}, & \lambda_a^{23} &= \frac{1}{\sqrt{2}\hbar^2}(\hbar S_y - \{S_y, S_z\}), \\
\lambda^1 &= 2\mathbb{1} + \frac{1}{2\hbar^2}\left(\hbar S_z - 3S_x^2 - 3S_y^2\right), & \lambda^2 &= \frac{1}{\sqrt{3}}\left(-2\mathbb{1} + \frac{3}{2\hbar^2}\left(\hbar S_z + S_x^2 + S_y^2\right)\right).
\end{aligned} \tag{75}$$

All operators can be represented by the following matrices:

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}, \qquad S_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&-\mathrm{i}&0\\\mathrm{i}&0&-\mathrm{i}\\0&\mathrm{i}&0\end{pmatrix}, \qquad S_z = \hbar\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix},$$

$$S_x^2 = \frac{\hbar^2}{2}\begin{pmatrix}1&0&1\\0&2&0\\1&0&1\end{pmatrix}, \qquad S_y^2 = \frac{\hbar^2}{2}\begin{pmatrix}1&0&-1\\0&2&0\\-1&0&1\end{pmatrix},$$

$$\{S_x, S_y\} = \hbar^2 \begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix}, \qquad \{S_y, S_z\} = \frac{\hbar^2}{\sqrt{2}} \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & \mathrm{i} \\ 0 & -\mathrm{i} & 0 \end{pmatrix},$$

$$\{S_z, S_x\} = \frac{\hbar^2}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}. \tag{76}$$

Thus we can express any observable on a n-qutrit Hilbert space—a composite system of n particles with 3 degrees of freedom—in terms of above spin operators (76).

As an example we want to study the entanglement witness for the isotropic two-qutrit state, i.e. state (40) for $d = 3$. In this case we obtain for the optimal entanglement witness

$$A_{\mathrm{iso}} = \tfrac{1}{3\sqrt{2}}\left(\mathbb{1} \otimes \mathbb{1} - \tfrac{3}{4}\Lambda\right), \tag{77}$$

(i.e. equation (67) for $d = 3$), where the operator Λ is defined in equation (49).

Expressing the Gell–Mann matrices in Λ (49) by the spin operator decomposition (75) we find for the expectation value of the entanglement witness A_{iso}

$$\langle A_{\mathrm{iso}}\rangle = \tfrac{1}{3\sqrt{2}}\langle \mathbb{1} \otimes \mathbb{1}\rangle - \tfrac{1}{4\sqrt{2}}\langle \Lambda \rangle, \tag{78}$$

where

$$\begin{aligned} \langle \Lambda \rangle = {} & \frac{1}{\hbar^2}(\langle S_x \otimes S_x\rangle - \langle S_y \otimes S_y\rangle + \langle S_z \otimes S_z\rangle) + \frac{16}{3}\langle \mathbb{1} \otimes \mathbb{1}\rangle \\ & - \frac{4}{\hbar^2}\left(\left\langle \mathbb{1} \otimes S_x^2\right\rangle + \left\langle \mathbb{1} \otimes S_y^2\right\rangle + \left\langle S_x^2 \otimes \mathbb{1}\right\rangle + \left\langle S_y^2 \otimes \mathbb{1}\right\rangle\right) \\ & + \frac{4}{\hbar^4}\left(\left\langle S_x^2 \otimes S_x^2\right\rangle + \left\langle S_y^2 \otimes S_y^2\right\rangle\right) + \frac{2}{\hbar^4}\left(\left\langle S_x^2 \otimes S_y^2\right\rangle + \left\langle S_y^2 \otimes S_x^2\right\rangle\right) \\ & + \frac{1}{\hbar^4}(\langle \{S_z, S_x\} \otimes \{S_z, S_x\}\rangle - \langle \{S_y, S_z\} \otimes \{S_y, S_z\}\rangle - \langle \{S_x, S_y\} \otimes \{S_x, S_y\}\rangle). \end{aligned} \tag{79}$$

Decomposition (79) has to be determined experimentally by measuring the several expectation values with the set-ups on both Alice's and Bob's side.

The advantage of the entanglement witness procedure is that for an experimental outcome $\langle A_{\mathrm{iso}}\rangle < 0$ the considered quantum state is definitely entangled, whereas in the case of Bell inequalities a violation detects *nonlocal* states. That means by the entanglement witness procedure we are able to detect more entangled states than with Bell inequalities. The amount of measurement steps necessary to determine an entanglement witness is about the same as in the Bell inequality procedure (see, e.g., [28–31]).

8. Conclusion

In this paper we present three different matrix bases which are quite useful to decompose density matrices for higher-dimensional qudits. These are the generalized Gell–Mann matrix basis, the polarization operator basis and the Weyl operator basis. Each decomposition we identify with a vector, the so-called Bloch vector.

Considering just one-particle states we observe the following features: the generalized Gell–Mann matrix basis is easy to construct, the matrices correspond to the standard SU(N) generators ($N = d$), but in general (in d dimensions) it is rather unpractical to work with the diagonal matrices (5) due to their more complicated definition. On the other hand, the Bloch vector itself has real components, which is advantageous, they can be expressed as expectation values of measurable quantities. For example, in three dimensions the Gell–Mann matrices are Hermitian and the Bloch vector components can be expressed by expectation values of spin-1 operators. The polarization operator basis is also easy to set up, all you need to know are the Clebsch–Gordan coefficients which you find tabulated in the literature. However, the Bloch vector contains complex components. For the Weyl operator basis the corresponding operators are again simple to construct, they are non-Hermitian but unitary. The Bloch vector itself has a very simple structure, however, with complex components. Let us note that in two dimensions all bases are equivalent since they correspond to Pauli matrices or linear combinations thereof.

In the case of two-qudits we have studied the isotropic states explicitly and find the following: in the generalized Gell–Mann matrix basis the Bloch vector (48) with expression (49) is more complicated to construct, in particular the diagonal part B (46) (see appendix A.2). In the polarization operator basis the Bloch vector (53) with expression (52) can easily be set up by knowledge of the Clebsch–Gordon coefficient sum rule (50) and in the Weyl operator basis the Bloch vector (56) with definition (55) is actually most easily to construct.

The Hilbert–Schmidt measure of entanglement can be calculated explicitly for all isotropic two-qudit states and we want to emphasize its interesting connection to the maximal violation of the entanglement witness inequality, theorem 1.

For the experimental realization of an entanglement witness the generalized Gell–Mann matrix basis is the appropriate one since the generalized Gell–Mann matrices are Hermitian. For a different task, however, the determination of the geometry of entanglement the Weyl operator basis turns out to be optimal. In our example of the entangled isotropic two-qutrit state the entanglement witness can be expressed by experimental quantities, the expectation values of spin-1 measurements. In this way one can experimentally find out whether a state is entangled or not, i.e. we can obtain rather precise information on the quality of entanglement.

Quite generally, the Bloch vector decomposition into one of the three matrix bases is of particular advantage in the construction of entanglement witnesses. It turns out that if the coefficients of the decomposition satisfy a certain condition the considered operator represents an entanglement witness, i.e. satisfies inequalities (58) (for details see [32]).

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Appendix

A.1. Proof of orthogonality of GGB

We want to prove condition (1) for the GGB which consists of the $d^2 - 1$ GGM (3)–(5) and the $d \times d$ unity $\mathbb{1}$. Since all GGM are Hermitian (thus $\mathrm{Tr}\, A_i^\dagger A_j = \mathrm{Tr}\, A_i A_j = \mathrm{Tr}\, A_j A_i$) it suffices to prove the following conditions:

$$\mathrm{Tr}\, \Lambda_s^{jk} \Lambda_s^{mn} = 2\delta^{jm}\delta^{kn} \tag{A.1}$$

$$\mathrm{Tr}\, \Lambda_a^{jk} \Lambda_a^{mn} = 2\delta^{jm}\delta^{kn} \tag{A.2}$$

$$\mathrm{Tr}\, \Lambda^{l} \Lambda^{m} = 2\delta^{lm} \tag{A.3}$$

$$\mathrm{Tr}\, \Lambda_a^{jk} \Lambda_s^{mn} = 0 \tag{A.4}$$

$$\mathrm{Tr}\,\Lambda_s^{jk}\Lambda^m = 0 \tag{A.5}$$

$$\mathrm{Tr}\,\Lambda_a^{jk}\Lambda^m = 0. \tag{A.6}$$

Proof of condition (A.1). Inserting definition (3) we have

$$\begin{aligned}\mathrm{Tr}\,\Lambda_s^{jk}\Lambda_s^{mn} &= \sum_{l=1}^{d}\langle l|(|j\rangle\langle k| + |k\rangle\langle j|)(|m\rangle\langle n| + |n\rangle\langle m|)|l\rangle \\ &= \sum_{l}(\langle l|j\rangle\langle k|m\rangle\langle n|l\rangle + \langle l|j\rangle\langle k|n\rangle\langle m|l\rangle + \langle l|k\rangle\langle j|m\rangle\langle n|l\rangle + \langle l|k\rangle\langle j|n\rangle\langle m|l\rangle) \\ &= \delta^{jn}\delta^{km} + \delta^{jm}\delta^{kn} + \delta^{kn}\delta^{jm} + \delta^{km}\delta^{jn} \\ &= 2\delta^{jm}\delta^{kn},\end{aligned} \tag{A.7}$$

where we used in the last step that $\delta^{jn}\delta^{km} = 0$ since we have $j < k$ *and* $m < n$.

Proof of condition (A.2). This case is equivalent to that before apart from changed signs that do not matter

$$\begin{aligned}\mathrm{Tr}\,\Lambda_a^{jk}\Lambda_a^{mn} &= -\delta^{jn}\delta^{km} + \delta^{jm}\delta^{kn} + \delta^{kn}\delta^{jm} - \delta^{km}\delta^{jn} \\ &= 2\delta^{jm}\delta^{kn}.\end{aligned} \tag{A.8}$$

Proof of condition (A.3). Using definition (5) and denoting

$$C_l = \sqrt{\frac{2}{l(l+1)}}, \tag{A.9}$$

where $l \leqslant m$ without loss of generality, we get

$$\begin{aligned}\mathrm{Tr}\,\Lambda^l\Lambda^m &= C_l C_m \sum_{p=1}^{d}\left(\sum_{k=1}^{l}\sum_{n=1}^{m}\langle p|k\rangle\langle k|n\rangle\langle n|p\rangle + lm\langle p|l+1\rangle\langle l+1|m+1\rangle\langle m+1|p\rangle\right. \\ &\quad \left. - m\sum_{k=1}^{l}\langle p|k\rangle\langle k|m+1\rangle\langle m+1|p\rangle - l\sum_{n=1}^{m}\langle p|l+1\rangle\langle l+1|n\rangle\langle n|p\rangle\right) \\ &= C_l C_m\left(l + lm\delta^{lm} - m\sum_{k=1}^{l}\delta^{k(m+1)} - l\sum_{n=1}^{m}\delta^{n(l+1)}\right).\end{aligned} \tag{A.10}$$

Using the fact that $\delta^{k(m+1)} = 0$ for $m \geqslant k$ and

$$l\sum_{n=1}^{m}\delta^{n(l+1)} = \begin{cases} 0 & \text{if} \quad l = m \\ l & \text{if} \quad l < m \end{cases} \tag{A.11}$$

we obtain

$$\mathrm{Tr}\,\Lambda^l\Lambda^m = (C_l)^2 l(l+1)\delta^{lm} = 2\delta^{lm}. \tag{A.12}$$

Proof of condition (A.4). Analogously to proofs (A.7) and (A.8) we find

$$\mathrm{Tr}\,\Lambda_a^{jk}\Lambda_s^{mn} = \mathrm{i}(-\delta^{jn}\delta^{km} + \delta^{jm}\delta^{kn} - \delta^{jm}\delta^{kn} + \delta^{jn}\delta^{km}) = 0. \tag{A.13}$$

Proof of condition (A.5). Inserting definitions (3) and (5) gives

$$\begin{aligned}\operatorname{Tr}\Lambda_s^{jk}\Lambda^m &= C_m \sum_{p=1}^{d}\Bigg(-m\langle p|k\rangle\langle j|m+1\rangle\langle m+1|p\rangle - m\langle p|j\rangle\langle k|m+1\rangle\langle m+1|p\rangle \\ &\quad + \sum_{n=1}^{m}\langle p|j\rangle\langle k|n\rangle\langle n|p\rangle + \sum_{n=1}^{m}\langle p|k\rangle\langle j|n\rangle\langle n|p\rangle\Bigg) \\ &= -2m\delta^{j(m+1)}\delta^{k(m+1)} + 2\sum_{l=1}^{m}\delta^{kl}\delta^{jl} \\ &= 0, \end{aligned} \tag{A.14}$$

since per definition we have $j < k$.

Proof of condition (A.6). This proof is equivalent to the previous one since constant factors in front of the terms do not matter.

A.2. Calculation of term B in GGB

To obtain the Bloch vector notation of term B (44) we insert the standard matrix expansion (14) for the case $j = k$. We split the tensor products in the following way:

$$B = \frac{1}{d}\left(B_1 + B_2 + B_3 + B_4 + \frac{1}{d}\mathbb{1}\otimes\mathbb{1}\right), \tag{A.15}$$

where the terms $B_1, \ldots, B_4$ are introduced by (note that $\Lambda^0 = 0$)

$$B_1 = \sum_{j=1}^{d}\left(\frac{j-1}{2j}\Lambda^{j-1}\otimes\Lambda^{j-1} + \sum_{n(=l)=0}^{d-j-1}\frac{1}{2(j+n)(j+n+1)}\Lambda^{j+n}\otimes\Lambda^{j+n}\right) \tag{A.16}$$

$$\begin{aligned} B_2 = \sum_{j=1}^{d}\Bigg(&-\sum_{l=0}^{d-j-1}\sqrt{\frac{j-1}{4j(j+l)(j+l+1)}}\Lambda^{j-1}\otimes\Lambda^{j+l} \\ &-\sum_{n=0}^{d-j-1}\sqrt{\frac{j-1}{4j(j+n)(j+n+1)}}\Lambda^{j+n}\otimes\Lambda^{j-1} \\ &+\sum_{n\neq l,n,l=0}^{d-j-1}\frac{1}{2\sqrt{(j+n)(j+n+1)(j+l)(j+l+1)}}\Lambda^{j+n}\otimes\Lambda^{j+l}\Bigg) \end{aligned} \tag{A.17}$$

$$B_3 = \frac{1}{d}\sum_{j=1}^{d}\left(-\sqrt{\frac{j-1}{2j}}\Lambda^{j-1}\otimes\mathbb{1} + \sum_{n=0}^{d-j-1}\frac{1}{\sqrt{2(j+n)(j+n+1)}}\Lambda^{j+n}\otimes\mathbb{1}\right) \tag{A.18}$$

$$B_4 = \frac{1}{d}\sum_{j=1}^{d}\left(-\sqrt{\frac{j-1}{2j}}\mathbb{1}\otimes\Lambda^{j-1} + \sum_{l=0}^{d-j-1}\frac{1}{\sqrt{2(j+l)(j+l+1)}}\mathbb{1}\otimes\Lambda^{j+l}\right). \tag{A.19}$$

Only the first term B_1 (A.16) gives a contribution

$$B_1 = \sum_{m=1}^{d-1}\left(\frac{m}{2(m+1)} + \frac{m}{2m(m+1)}\right)\Lambda^m\otimes\Lambda^m = \frac{1}{2}\sum_{m=1}^{d-1}\Lambda^m\otimes\Lambda^m, \tag{A.20}$$

whereas the remaining terms vanish:

$$\begin{aligned}
B_2 &= \sum_{m<p,m,p=1}^{d-1} \left(-\sqrt{\frac{m}{4(m+1)p(p+1)}} + \frac{m}{\sqrt{4m(m+1)p(p+1)}} \right) \Lambda^m \otimes \Lambda^p \\
&\quad + \sum_{m>p,m,p=1}^{d-1} \left(-\sqrt{\frac{p}{4(p+1)m(m+1)}} + \frac{p}{\sqrt{4p(p+1)m(m+1)}} \right) \Lambda^m \otimes \Lambda^p \\
&= \left(\sum_{m<p} \frac{-m+m}{2\sqrt{m(m+1)p(p+1)}} + \sum_{m>p} \frac{-p+p}{2\sqrt{m(m+1)p(p+1)}} \right) \Lambda^m \otimes \Lambda^p \\
&= 0,
\end{aligned} \tag{A.21}$$

and in quite the same manner

$$\begin{aligned}
B_3 &= \frac{1}{d} \sum_{m=1}^{d-1} \frac{-m+m}{\sqrt{2m(m+1)}} \Lambda^m \otimes \mathbb{1} = 0, \\
B_4 &= \frac{1}{d} \sum_{p=1}^{d-1} \frac{-p+p}{\sqrt{2p(p+1)}} \mathbb{1} \otimes \Lambda^p = 0.
\end{aligned} \tag{A.22}$$

Thus we find the following Bloch vector of B (44):

$$B = \frac{1}{2d} \sum_{m=1}^{d-1} \Lambda^m \otimes \Lambda^m + \frac{1}{d^2} \mathbb{1} \otimes \mathbb{1}. \tag{A.23}$$

A.3. Proof of orthonormality of WOB

For proofs relevant in the WOB we often need the equivalence

$$\sum_{n=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} nx} = \begin{cases} d & \text{if} \quad x = 0 \\ 0 & \text{if} \quad x \neq 0, \end{cases} \qquad x \in \mathbb{Z}. \tag{A.24}$$

So we use equation (A.24) to prove orthonormality (31) of the Weyl operators (30)

$$\begin{aligned}
\operatorname{Tr} U_{nm}^{\dagger} U_{lj} &= \sum_{p=0}^{d-1} \sum_{k,\tilde{k}=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(\tilde{k}l - kn)} \langle p|(k+m) \bmod d\rangle \langle k|\tilde{k}\rangle \langle (\tilde{k}+j) \bmod d|p\rangle \\
&= \sum_{p=0}^{d-1} \sum_{k,\tilde{k}=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(\tilde{k}l - kn)} \langle p|(k+m) \bmod d\rangle \langle (\tilde{k}+j) \bmod d|p\rangle \delta_{k\tilde{k}} \\
&= \sum_{k=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} k(l-n)} \delta_{mj} \\
&= d\delta_{nl}\delta_{mj}.
\end{aligned} \tag{A.25}$$

A.4. Expansion into WOB

Formula (54) for the Bell state in terms of WOB we derive in the following way. We express the standard matrices by the WOB (37), rewrite the indices and separate the nonvanishing terms

$$
\begin{aligned}
|\phi_+^d\rangle\langle\phi_+^d| &= \frac{1}{d}\sum_{j,k=1}^{d} |j\rangle\langle k| \otimes |j\rangle\langle k| \\
&= \frac{1}{d^3}\sum_{j,k=0}^{d-1}\sum_{l,l'=0}^{d-1} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} j(l+l')} U_{l(k-j)\bmod d} \otimes U_{l'(k-j)\bmod d} \\
&= \frac{1}{d^3}\sum_{m,k=0}^{d-1}\sum_{l,l'=0}^{d-1} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d}(k-m)(l+l')} U_{lm} \otimes U_{l'm} \\
&= \frac{1}{d^2}\left(\sum_{m} U_{0m}\otimes U_{0m} + \sum_{m}\sum_{l,l';l+l'=d} U_{lm}\otimes U_{l'm}\right) \\
&\quad + \frac{1}{d^3}\sum_{m}\sum_{l,l';l,l'\neq 0,0;l+l'\neq d}\left(\sum_{k}\mathrm{e}^{-\frac{2\pi \mathrm{i}}{d}(k-m)(l+l')}\right) U_{lm}\otimes U_{l'm}.
\end{aligned} \tag{A.26}
$$

The last term in equation (A.26) vanishes due to relation (A.24). Identifying $U_{00} = \mathbb{1}$ and using the notation with negative values of the index l, which have to be considered as mod d, we gain the formula

$$
|\phi_+^d\rangle\langle\phi_+^d| = \frac{1}{d^2}\mathbb{1}\otimes\mathbb{1} + \frac{1}{d^2}\sum_{l,m=0}^{d-1} U_{lm}\otimes U_{-lm}, \qquad (l,m)\neq(0,0). \tag{A.27}
$$

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