The generalized Gell-Mann representation and violation of the CHSH inequality by a general two-qudit state

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Abstract

We formulate and prove the main properties of the generalized Gell-Mann representation for traceless qudit observables and analyze via this representation violation of the CHSH inequality by a general two-qudit state. For the maximal CHSH violation by a two-qudit state with an arbitrary qudit dimension $d \geq 2$, this allows us to derive two new bounds, lower and upper, which are expressed via the spectral properties of the correlation matrix for a two-qudit state. We have not yet been able to specify a class of two-qudit states for which the new upper bound improves the general upper bound of Tsirelson. However, this is the case for each two-qubit state, where the new lower bound and the new upper bound coincide and reduce to the precise two-qubit CHSH result of Horodecki, and also, for the Greenberger–Horne–Zeilinger (GHZ) state with an arbitrary odd qudit dimension $d \geq 2$, where the new upper bound is less than the upper bound of Tsirelson. Moreover, we explicitly find the correlation matrix for the GHZ state and prove that, for this state, the new upper bound is attained for each $d \geq 2$ and this specifies the following new result: the maximal violation of the CHSH inequality by the two-qudit GHZ state is equal to $\sqrt{2}$ if a qudit dimension $d \geq 2$ is even and to $\frac{d+1}{d}\sqrt{2}$ if a qudit dimension $d \geq 2$ is odd.

1 Introduction

Different aspects of quantum violation of the Clauser-Horne-Shimony-Holt (CHSH) inequality [1] were studied since 1969 in a huge number of papers (see [2, 3, 4, 5, 6, 7, 8] and references therein).

It is well known due to Tsirelson [3, 4] that, for all bipartite quantum states, the maximal violation of the CHSH inequality cannot exceed the (Tsirelson) upper bound $\sqrt{2}$ and that this upper bound is attained on the two-qubit Bell states.

It is also well known that, for the maximal violation of the CHSH inequality by an arbitrary two-qubit state, Horodecki [6] found the precise value specified via the correlation properties of this two-qubit state.
However, for a general two-qudit state with an arbitrary qudit dimension $d > 2$, bounds on the maximal CHSH violation in terms of the correlation properties of this state have not been analyzed.

In the present paper, we formulate and prove the main properties of the generalized Gell-Mann representation for traceless qudit observables and study via this representation violation of the CHSH inequality for a general two-qudit state.

For the maximal violation of the CHSH inequality by a two-qudit state with an arbitrary qudit dimension $d \geq 2$, we find two new bounds, lower and upper, which are expressed via the spectral properties of the correlation matrix of this two-qudit state.

We have not yet been able to specify a class of two-qudit states for which the new upper bound improves the general upper bound of Tsirelson \[3, 4\]. However, this is the case for each two-qubit state, where the new lower bound and the new upper bound coincide and reduce to the precise two-qubit result of Horodecki in \[6\], and also, for the two-qudit Greenberger–Horne–Zeilinger (GHZ) state with an arbitrary odd $d \geq 2$, where the new upper bound is less than the Tsirelson upper bound \[3, 4\].

Applying our new general results for the Greenberger–Horne–Zeilinger (GHZ) state with an arbitrary $d \geq 2$, we explicitly find the eigenvalues of the correlation matrix for this state and prove that, for the two-qudit GHZ state, the new upper bound is attained for each $d \geq 2$ and specifies the precise value of its maximal CHSH violation: $\sqrt{2}$ if a dimension $d \geq 2$ is even and $\frac{d-1}{d} \sqrt{2}$ if a dimension $d \geq 2$ is odd.

The paper is organized as follows.

In Section 2, we formulate and prove (Proposition 1) the main properties of the generalized Gell-Mann representation for traceless qudit observables.

In Section 3, via the properties of the generalized Gell-Mann representation proved in Section 2, we study violation of the CHSH inequality in a general two-qudit case and derive new bounds (Theorem 1) on the maximal CHSH violation by a two-qudit state with an arbitrary $d \geq 2$.

In Section 4, we show that, for the GHZ state, the new upper bound is less (Proposition 2) than the Tsirelson upper bound and prove (Theorem 2) that, for the two-qudit GHZ state, the new upper bound is attained for each $d \geq 2$.

In Section 5, we summarize the main new results of the present paper.

## 2 Representation of traceless qudit observables

For an arbitrary observable $Y$ on $\mathbb{C}^d$, $d \geq 2$, the generalized Gell–Mann representation (see e. g. in \[9, 10, 11\]) reads:

$$ Y = \alpha \mathbb{I} + n \cdot \Lambda, \quad n \cdot \Lambda := \sum_{j=1, \ldots, d^2-1} n_j \Lambda_j, \quad (1) $$

$$ \alpha = \frac{1}{d} \text{tr}[Y], \quad n_j = \frac{1}{2} \text{tr}[Y \Lambda_j], $$

$$ 2 $$
where \( n \) is a vector in \( \mathbb{R}^{d^2-1} \) and \( \Lambda_j, j = 1, \ldots, d^2 - 1 \), are traceless hermitian operators on \( \mathbb{C}^d \) (generators of \( SU(d) \) group), satisfying the relation
\[
\text{tr}[\Lambda_j \Lambda_{j1}] = 2\delta_{jj_1}.
\] (2)

The tuple \( \Lambda := (\Lambda_1, \ldots, \Lambda_{d^2-1}) \) of these traceless hermitian operators has the following form
\[
(\Lambda_{12}^{(s)}, \ldots, \Lambda_{ld}^{(s)}, \Lambda_{d-1,d}^{(as)}, \ldots, \Lambda_{ld}^{(as)}, \Lambda_1^{(d)}, \ldots, \Lambda_{d-1}^{(d)}),
\] (3)

where
\[
\Lambda_{mk}^{(s)} = |m\rangle \langle k| + |k\rangle \langle m|, \quad \Lambda_{mk}^{as} = \Lambda_{km}^{as}, \quad 1 \leq m < k \leq d,
\] (4)
\[
\Lambda_{mk}^{(as)} = -i |m\rangle \langle k| + i |k\rangle \langle m|, \quad \Lambda_{mk}^{as} = -\Lambda_{km}^{as}, \quad 1 \leq m < k \leq d
\] (5)
\[
\Lambda_l^{(d)} = \sqrt{\frac{2}{l(l+1)}} \left( \sum_{j=1}^{d-l} |j\rangle \langle j| - t |l+1\rangle \langle l+1| \right), \quad 1 \leq l \leq d-1,
\] (6)

and \( \{|j\rangle \in \mathbb{C}^d, j = 1, \ldots, d\} \) is the computational basis of \( \mathbb{C}^d \).

Representation (1) constitutes decomposition of a qudit observable \( Y \) in the orthonormal basis \( \{I, \Lambda_j, j = 1, \ldots, d^2 - 1\} \) of the Hilbert–Schmidt Hilbert space where qudit observables are vectors and the scalar product is defined via \( \langle Y, Y' \rangle_{\text{sch}} := \text{tr}[YY'] \).

The matrix representations of operators \( \Lambda_i, i = 1, \ldots, d^2 - 1 \) in the computational basis of \( \mathbb{C}^d \) constitute the higher-dimensional extensions of the Pauli matrices for qubits \( (d = 2) \) and the Gell–Mann matrices for qutrits \( (d = 3) \).

For a traceless qudit observable \( X \), representation (1) takes the form
\[
X = n \cdot \Lambda, \quad n_j = \frac{1}{2} \text{tr}[X \Lambda_j],
\] (7)
and implies
\[
\text{tr}[X^2] = 2 \|n\|^2.
\] (8)

The following statement is proved in Appendix A.

**Lemma 1** For each \( n \in \mathbb{R}^{d^2-1} \) and each \( d \geq 2 \),
\[
\sqrt{\frac{2}{d}} \leq \frac{\|n \cdot \Lambda\|_0}{\|n\|} \leq \sqrt{\frac{2(d-1)}{d}} \leq \sqrt{\frac{2}{1 + \delta_{d^2}}},
\] (9)

where (i) notation \( \|\cdot\|_0 \) means the operator norm of an observable on \( \mathbb{C}^d \) and \( \|\cdot\| \) – the Euclidian norm of a vector \( n \) in \( \mathbb{R}^{d^2-1} \); (ii) \( \delta_{d^2} = 1 \) for \( d = 2 \) and \( \delta_{d^2} = 0 \), otherwise.

From the lower bound in (9) it follows that, for each \( n \in \mathbb{R}^{d^2-1} \), relation \( \|n \cdot \Lambda\|_0 \leq \sqrt{\frac{2}{d}} \) implies \( \|n\| \leq 1 \), and if \( \|n \cdot \Lambda\|_0 \leq \sqrt{\frac{2}{d}} \|n\| \), then \( \|n \cdot \Lambda\|_0 = \sqrt{\frac{2}{d}} \|n\| \).
Remark 1 In the qubit case \((d = 2)\), operators \(\Lambda_j, \ j = 1, 2, 3\), constitute the Pauli operators \(\sigma_j, j = 1, 2, 3\), and bounds (9) reduce to the well-known relation
\[
\frac{\|n \cdot \sigma\|_0}{\|n\|} \big|_{d=2} = 1, \quad n \in \mathbb{R}^3,
\]
valid for any traceless qubit observable \(n \cdot \sigma\) – projection of the qubit spin on a direction \(n\) in \(\mathbb{R}^3\).

In what follows, we use the following notations, for short.

Definition 1 Denote by \(L_d\) the set of all traceless qudit observables on \(\mathbb{C}^d\) with eigenvalues in \([-1, 1]\) and by \(L_d^{(s)} \subset L_d\) the subset of all traceless qudit observables \(\tilde{X}_s\) with a dimension\(^1\) \(s \geq 0\) of their kernels and all their eigenvalues in set \([-1, 0, 1]\). Subset \(L_d^{(0)} \neq \emptyset\) iff a dimension \(d \geq 2\) is even.

Normalizing a vector \(n\) in decomposition (7) in view of the lower bound in (9), we represent each traceless qudit observable \(X \in L_d\) in the form
\[
X = \sqrt{\frac{d}{2}} \left( n_X \cdot \Lambda \right), \quad n_X^{(j)} = \frac{1}{\sqrt{2d}} \text{tr}[X \Lambda_j], \quad n_X \in \mathbb{R}^{d^2-1},
\]
so that, under representation (11),
\[
\|X\|_0 \leq 1 \iff \|n_X \cdot \Lambda\|_0 \leq \sqrt{\frac{2}{d}}.
\]
Therefore, representation (11) establishes the mapping
\[
\Phi : L_d \rightarrow \mathfrak{R}_d
\]
of all traceless observables in \(L_d\) to vectors \(n \in \mathbb{R}^{d^2-1}\) in the set
\[
\mathfrak{R}_d = \left\{ n \in \mathbb{R}^{d^2-1} \mid \|n \cdot \Lambda\|_0 \leq \sqrt{\frac{2}{d}} \right\}
\]
and since (11) constitutes the decomposition via the basis \(\{I, \Lambda_j, j = 1, \ldots, d^2 - 1\}\) of the Hilbert-Schmidt Hilbert space, the mapping \(\Phi\) is injective.

Under representation (11), for all observables \(X \in L_d^{(s)}\),
\[
\text{tr}[X^2] = (d - s) = d \|n_X\|^2.
\]

\(^1\)If \(s > 0\), then it constitutes the multiplicity of the zero eigenvalue of an observable in \(L_d^{(s)}\).
Therefore, all traceless observables in $L_d^{(s)} \subset L_d$, $s \geq 0$, are mapped to vectors $n$ in

$$\mathcal{R}_d^{(s)} = \left\{ n \in \mathbb{R}^{d^2-1} \mid \|n \cdot \Lambda\|_0 = \sqrt{\frac{2}{d}} \|n\| = \sqrt{\frac{d - s}{d}} \right\} \subset \mathbb{R}_d, \quad s \geq 0. \quad (17)$$

In particular, all traceless qudit observables with eigenvalues $\pm 1$ (i.e. in subset $L_d^{(0)} \subset L_d$), are mapped to vectors in

$$\mathcal{R}_d^{(0)} = \left\{ n \in \mathbb{R}^{d^2-1} \mid \|n \cdot \Lambda\|_0 = \sqrt{\frac{2}{d}} \|n\| = 1 \right\} \subset \mathbb{R}_d. \quad (18)$$

Conversely, let $n$ be an arbitrary vector in set $\mathcal{R}_d$, defined by (15). For the traceless qudit observable, corresponding to each $n \in \mathcal{R}_d$, via the representation $X_n = \sqrt{\frac{d}{2}} (n \cdot \Lambda), \quad \text{tr}[X_n^2] = d \|n\|^2$, the operator norm $\|X_n\|_0 \leq 1$ and, therefore, $X_n \in L_d$. Hence, the injective mapping (14) is surjective, therefore, bijective.

Furthermore, let subset $\mathcal{R}_d^{(0)} \subset \mathcal{R}_d$, given by (18), be not empty and $r \in \mathcal{R}_d^{(0)}$ be a unit vector in this subset. For the observable $X_r = \sqrt{\frac{2}{d}} r \cdot \Lambda$ in $L_d$ corresponding to a unit vector $r \in \mathcal{R}_d^{(0)}$ via (19), we have

$$\|X_r\|_0 = 1, \quad \text{tr}[X_r^2] = d. \quad (20)$$

But this is possible iff $X_r \in L_d^{(0)}$. Therefore, representation (19) establishes the one-to-one correspondence between observables in the subset $L_d^{(0)} \subset L_d^{(0)}$ and vectors in the intersection $\mathcal{R}_d^{(0)}$ of $\mathcal{R}_d$ with the unit sphere. Since $L_d^{(0)} \neq \emptyset$ iff a dimension $d \geq 2$ is even, also, subset $\mathcal{R}_d^{(0)} \neq \emptyset$ iff a dimension $d \geq 2$ is even.

Let us now analyze geometry of set $\mathcal{R}_d$, $d \geq 2$, defined by (15).

As specified in Remark 1, in the qubit ($d = 2$) case, for each $n \in \mathbb{R}^3$, the norm $\|n \cdot \sigma\|_0 = \|n\|$. Therefore, in (15), relation $\|n \cdot \Lambda\|_0 \leq 1$ is equivalent to $\|n\| \leq 1$, the set

$$\mathcal{R}_2 = \left\{ n \in \mathbb{R}^3 \mid \|n\| \leq 1 \right\} \quad (21)$$

costitutes the unit ball in $\mathbb{R}^3$.

Due to (15), for each vector $n \in \mathcal{R}_d$ along $j$-th coordinate axis in $\mathbb{R}^{d^2-1}$, the norm cannot exceed

$$\sqrt{\frac{2}{d}} \frac{1}{\|A_j\|_{op}}, \quad j = 1, \ldots, d^2 - 1, \quad (22)$$

where the operator norms of all observables (11) and (15) are equal to 1, whereas the operator norms of observables (16) vary from 1 to $\sqrt{\frac{2(d-1)}{d}}$. Therefore, the lengths (22) of
vectors along different coordinate axes in $\mathbb{R}^{d^2-1}$ vary from $\sqrt{\frac{2}{d}}$ to $\sqrt{\frac{1}{d-1}}$ and are equal to each other if only $d = 2$. Thus, for $d > 2$, the form of the bounded set $\mathfrak{K}_d$ with respect to different axes is asymmetric.

The maximal norm $l_d := \max_{n \in \mathfrak{K}_d} \|n\|$ of a vector $n \in \mathfrak{K}_d$ is calculated via (12):

$$l_d := \max_{n \in \mathfrak{K}_d} \|n\| = \sqrt{\frac{1}{d} \max_{X \in \mathcal{L}_d} \text{tr}[X^2]} = \sqrt{\frac{1}{d} \max_{\lambda_m \in D} \sum_m \lambda_m^2},$$

(23)

and is equal to

$$l_d = 1, \quad \text{if } d \geq 2 \text{ is even},$$

(24)

$$l_d = \sqrt{\frac{d-1}{d}}, \quad \text{if } d \geq 2 \text{ is odd}.$$ 

In (23), $\{\lambda_m \in [-1,1], m = 1, \ldots, d\}$ are eigenvalues of a traceless observable $X = \sqrt{\frac{2}{d}} (n \cdot \Lambda) \in \mathcal{L}_d$ and $D = \{ |\lambda_m| \leq 1 \mid \sum_m \lambda_m = 0 \}$.

For an even $d \geq 2$, the maximal norm $l_d$ is attained on vectors $n \in \mathfrak{K}_d^{(0)}$, corresponding to observables in $\mathcal{L}_d^{(0)}$, for an odd $d \geq 2$ on vectors $n \in \mathfrak{K}_d^{(1)}$, corresponding to observables in $\mathcal{L}_d^{(1)}$ (see Definition 1).

From (23) it follows, that, for all $n \in \mathfrak{K}_d$, the norms

$$\|n\| \leq l_d \leq 1,$$

(25)

so that $\mathfrak{K}_d$ is a subset of the ball in $\mathbb{R}^{d^2-1}$ of radius $l_d \leq 1$. Relations (9), (15) imply that

$$\mathfrak{K}_d \supseteq \left\{ n \in \mathbb{R}^{d^2-1} \mid \|n\| = \sqrt{\frac{1}{d-1}} \right\},$$

(26)

therefore, $\mathfrak{K}_d$ contains the ball of radius $\sqrt{\frac{1}{d-1}}$. Note also that, for each vector $n \in \mathbb{R}^{d^2-1}$, the vector

$$\tilde{n} = \frac{\sqrt{d}}{d} n \|n \cdot \Lambda\|_0 \in \mathfrak{K}_d.$$ 

(27)

Summing up, we have proved the following statement.

**Proposition 1 Representation**

$$X = \sqrt{\frac{d}{2}} (n \cdot \Lambda)$$

(28)

establishes the one-to-one correspondence $\mathcal{L}_d \leftrightarrow \mathfrak{K}_d$ between traceless qudit observables $X$ with eigenvalues in $[-1,1]$ and vectors $n$ in the set $\mathfrak{K}_d$, defined by (15) and having, in general, the complicated form specified above by (21)–(27). The maximal norm $l_d$ of a vector in $\mathfrak{K}_d$ is equal to 1 if a qudit dimension $d \geq 2$ is even and to $\sqrt{\frac{d-1}{d}}$, if a qudit
dimension $d \geq 2$ is odd. Under the one-to-one correspondence $\mathcal{L}_d \leftrightarrow \mathcal{R}_d$ established by (28), sets

$$\mathcal{L}_d^{(0)} \leftrightarrow \mathcal{R}_d^{(0)} = \{ n \in \mathcal{R}_d \mid \|n\| = 1 \}$$

and are not empty iff a dimension $d \geq 2$ is even.

In the next section, we use Proposition 1 for analyzing violation of the CHSH inequality by an arbitrary two-qudit state.

**3 Violation of the CHSH inequality by a two-qudit state**

Let $\rho_{d \times d}$ be a state on $\mathbb{C}^d \otimes \mathbb{C}^d$ and $A_i, B_k$, $i, k = 1, 2$, be traceless observables on $\mathbb{C}^d$ with eigenvalues in $[-1, 1]$, that is, $A_i, B_k \in \mathcal{L}_d$ (see Definition 1). In a quantum case, the Bell operator, associated with the CHSH inequality, is given by

$$B_{\text{chsh}}(A_1, A_2; B_1, B_2) = A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2)$$

(30)

and, for a state $\rho_{d \times d}$, the left-hand side of the CHSH inequality reads

$$\left| \text{tr}[\rho_{d \times d} B_{\text{chsh}}(A_1, A_2; B_1, B_2)] \right| = \left| \text{tr}[\rho_{d \times d}(A_1 \otimes (B_1 + B_2))] + \text{tr}[\rho_{d \times d}(A_2 \otimes (B_1 - B_2))] \right| .$$

(31)

For the expectation (31) of the Bell operator (30) in a state $\rho_{d \times d}$, let us analyze the least upper bound

$$\sup_{A_i, B_k \in \mathcal{L}_d} \left| \text{tr}[\rho_{d \times d} B_{\text{chsh}}(A_1, A_2; B_1, B_2)] \right|$$

(32)

over observables $A_i, B_k \in \mathcal{L}_d$.

For qudit observables $A_i, B_k \in \mathcal{L}_d$, representation (28) reads

$$A_i = \sqrt{\frac{d}{2}} (a_i \cdot \Lambda), \quad B_k = \sqrt{\frac{d}{2}} (b_k \cdot \Lambda), \quad a_i, b_k \in \mathcal{R}_d \subset \mathbb{R}^{d^2 - 1},$$

(33)

where set $\mathcal{R}_d$ is given by (15). Due to (33), each expectation $\text{tr}[\rho_{d \times d} \{ A_i \otimes B_k \}]$ in (31) is expressed via

$$\text{tr}[\rho_{d \times d} \{ A_m \otimes B_k \}] = \frac{d}{2} \sum_{n, m} a_m^{(i)} T_{d \times d}^{(ij)} b_k^{(j)}$$

(34)

$$= \frac{d}{2} \langle a_m, T_{d \times d} b_k \rangle,$$

where $T_{d \times d}$ is the linear operator on $\mathbb{R}^{d^2 - 1}$, defined in the standard basis of $\mathbb{R}^{d^2 - 1}$ by the two-qudit correlation matrix with real elements:

$$T_{d \times d}^{(ij)} := \text{tr}[\rho_{d \times d} \{ A_i \otimes A_j \}], \quad i, j = 1, \ldots, d^2 - 1.$$  

(35)

In the local hidden variable (LHV) model, the expectation $|\langle B_{\text{chsh}} \rangle_{\text{LHV}}| \leq 2$ – the CHSH inequality.
This \((d^2 - 1) \times (d^2 - 1)\) matrix constitutes a generalization to higher dimensions of the two-qubit correlation matrix, considered, for example, in [6] [11]. If a state \(\rho_{d \times d}\) is symmetric\(^3\), then \(T_{\rho_{d \times d}}\) is hermitian.

Substituting (34) into (31), we have

\[
\text{tr}[\rho_{d \times d} B_{\text{chsh}}(A_1, A_2; B_1, B_2)] = \frac{d}{2} \left\{ \langle a_1, T_{\rho_{d \times d}}(b_1 + b_2) \rangle + \langle a_2, T_{\rho_{d \times d}}(b_1 - b_2) \rangle \right\}. \tag{36}
\]

Due to the one-to-one correspondence \(L_d \leftrightarrow \mathcal{R}_d\) (see Proposition 1) between traceless qudit observables with eigenvalues in \([-1, 1]\) and vectors in the subset \(\mathcal{R}_d\) of \(\mathbb{R}^{d^2 - 1}\) given by (15), relation (36) implies

\[
\sup_{A_1, B_1 \in L_d} |\text{tr}[\rho_{d \times d} B_{\text{chsh}}(A_1, A_2; B_1, B_2)]| = \frac{d}{2} \sup_{a_1, b_1 \in \mathcal{R}_d} \left| \langle a_1, T_{\rho_{d \times d}}(b_1 + b_2) \rangle + \langle a_2, T_{\rho_{d \times d}}(b_1 - b_2) \rangle \right|. \tag{37}
\]

Taking into account continuity in \(a_i, b_i\) of scalar products on \(\mathbb{R}^{d^2 - 1}\), boundedness and closure of set \(\mathcal{R}_d\) and that \(L_d \leftrightarrow \mathcal{R}_d\), we have

\[
\sup_{A_1, B_1 \in L_d} |\text{tr}[\rho_{d \times d} B_{\text{chsh}}(A_1, A_2; B_1, B_2)]| = \frac{d}{2} \sup_{a_1, b_1 \in \mathcal{R}_d} \left| \langle a_1, T_{\rho_{d \times d}}(b_1 + b_2) \rangle + \langle a_2, T_{\rho_{d \times d}}(b_1 - b_2) \rangle \right|. \tag{38}
\]

Note since \(|\text{tr}[\rho_{d \times d} \{A \otimes B\}]| \leq 1\) for any state \(\rho_{d \times d}\) and all observables \(A, B \in L_d\), relation (34) implies

\[
|\langle a, T_{\rho_{d \times d}} b \rangle| \leq \frac{2}{d} \quad \text{for all } a, b \in \mathcal{R}_d. \tag{39}
\]

In the second line of (38), the maximum over \(a_i \in \mathcal{R}_d, i = 1, 2\), is attained on vectors

\[
\tilde{a}_1 = \sqrt{\frac{2}{d}} \frac{T_{\rho_{d \times d}}(b_1 + b_2)}{\|T_{\rho_{d \times d}}(b_1 + b_2) \cdot \Lambda\|_0} \in \mathcal{R}_d, \quad \tilde{a}_2 = \sqrt{\frac{2}{d}} \frac{T_{\rho_{d \times d}}(b_1 - b_2)}{\|T_{\rho_{d \times d}}(b_1 - b_2) \cdot \Lambda\|_0} \in \mathcal{R}_d, \tag{40}
\]

which are not necessarily unit, and it is equal to

\[
\sqrt{\frac{d}{2}} \left( \frac{\|T_{\rho_{d \times d}}(b_1 + b_2)\|^2}{\|T_{\rho_{d \times d}}(b_1 + b_2) \cdot \Lambda\|_0} + \frac{\|T_{\rho_{d \times d}}(b_1 - b_2)\|^2}{\|T_{\rho_{d \times d}}(b_1 - b_2) \cdot \Lambda\|_0} \right). \tag{41}
\]

Noting further that by (15), for arbitrary \(b_1, b_2 \in \mathcal{R}_d\), vectors \(\frac{b_1 + b_2}{2}\) are also in \(\mathcal{R}_d\), we generalize the calculation method used in [6] and introduce two vectors \(r_1, r_2 \in \mathcal{R}_d\), not

\(^3\text{In the sense that } \rho \text{ is invariant under permutation of spaces } \mathbb{C}^d \text{ in the tensor product } \mathbb{C}^d \otimes \mathbb{C}^d.\)
necessarily mutually orthogonal, satisfying the relations
\[
\frac{b_1 + b_2}{2} = r_1 \cos \theta, \quad \frac{b_1 - b_2}{2} = r_2 \sin \theta, \quad \theta \in [0, \pi/2],
\]  
(42)

\[2 \langle r_1, r_2 \rangle \sin 2\theta = \|b_1\|^2 - \|b_2\|^2.
\]

Substituting (42) into (41) and (41) into (38), we have
\[
\text{we have the bound}
\]

\[\theta
\]

where the maximum over \(\theta\) and is given by
\[
\frac{d}{2} \max_{a_i, b_k \in \mathcal{R}_d} \left| \langle a_1, T_{d \times d}(b_1 + b_2) \rangle + \langle a_2, T_{d \times d}(b_1 - b_2) \rangle \right|
\]

\[
(43)
\]

\[= \sqrt{2d} \max_{\theta, r_1, r_2 \in \mathcal{R}_d} \left( \frac{\|T_{d \times d} r_1\|^2}{\|T_{d \times d} r_1 \cdot \Lambda\|^2_0} \cos \theta + \frac{\|T_{d \times d} r_2\|^2}{\|T_{d \times d} r_2 \cdot \Lambda\|^2_0} \sin \theta \right),
\]

where the maximum over \(\theta \in [0, \pi/2]\) is attained at
\[
\tan \theta_0 = \frac{\|T_{d \times d} r_2\|^2}{\|T_{d \times d} r_1\|^2} \frac{\|T_{d \times d} r_1 \cdot \Lambda\|^2_0}{\|T_{d \times d} r_2 \cdot \Lambda\|^2_0}
\]

\[
(44)
\]

and is given by
\[
\sqrt{\frac{\|T_{d \times d} r_1\|^4}{\|T_{d \times d} r_1 \cdot \Lambda\|^4_0} + \frac{\|T_{d \times d} r_2\|^4}{\|T_{d \times d} r_2 \cdot \Lambda\|^4_0}}.
\]

\[
(45)
\]

From (38)–(45) it follows
\[
\max_{A_i, B_k \in \mathcal{R}_d} \|\text{tr}[\rho_{d \times d} \mathcal{B}_{\text{chsh}} (A_1, A_2; B_1, B_2)]\|
\]

\[
(46)
\]

\[= \sqrt{2d} \max_{r_1, r_2 \in \mathcal{R}_d} \left[ \frac{\|T_{d \times d} r_1\|^4}{\|T_{d \times d} r_1 \cdot \Lambda\|^4_0} + \frac{\|T_{d \times d} r_2\|^4}{\|T_{d \times d} r_2 \cdot \Lambda\|^4_0} \right].
\]

Let us first show that the derived expression (46) for maximum (38) leads at once to the Tsirelson upper bound. Namely, due to property (27) and relation (39), specified with vectors
\[
a = \sqrt{\frac{2}{d}} \frac{T_{d \times d} r}{\|T_{d \times d} r \cdot \Lambda\|^2_0} \in \mathcal{R}_d,
\]

\[
b = r \in \mathcal{R}_d,
\]

we have the bound
\[
\frac{\|T_{d \times d} r\|^2}{\|T_{d \times d} r \cdot \Lambda\|^2_0} \leq \sqrt{\frac{2}{d}}, \quad \text{for all } r \in \mathcal{R}_d.
\]

\[
(48)
\]

Substituting (48) into (46), we have
\[
\max_{A_i, B_k \in \mathcal{R}_d} \|\text{tr}[\rho_{d \times d} \mathcal{B}_{\text{chsh}} (A_1, A_2; B_1, B_2)]\| \leq 2\sqrt{2}, \quad \forall \rho_{d \times d}, \quad d \geq 2,
\]

\[
(49)
\]
that is, the Tsirelson upper bound derived originally [3] in the other way.

Furthermore, the derived expression (46) for the maximal value of (31) allows us to introduce the following two new general bounds, lower and upper, see Appendix B for the proof.

Theorem 1 For an arbitrary two-qudit state \( \rho_{d \times d} \), with the correlation matrix \( T_{\rho_{d \times d}} \) defined by (35), the maximal value of the CHSH expectation (31) over all traceless qudit observables with eigenvalues in \([-1, 1]\) admits the bounds

\[
\frac{d}{d-1} \sqrt{\lambda_{\rho_{d \times d}} + \tilde{\lambda}_{\rho_{d \times d}}} \leq \max_{A_1, B_1, B_2 \in L_d} |\text{tr}[\rho_{d \times d} B_{\text{CHSH}}(A_1, A_2; B_1, B_2)]| \leq l_d^2 d \sqrt{\lambda_{\rho_{d \times d}} + \tilde{\lambda}_{\rho_{d \times d}}},
\]

(50)

where \( \lambda_{\rho_{d \times d}} \geq \tilde{\lambda}_{\rho_{d \times d}} \geq 0 \) are two greater eigenvalues, corresponding to two linear independent eigenvectors of the positive hermitian matrix \( T^\dagger_{\rho_{d \times d}} T_{\rho_{d \times d}} \), and \( l_d = d \) if a qudit dimension \( d \geq 2 \) is even and \( l_d = \sqrt{\frac{d-1}{d}} \) if a qudit dimension \( d \geq 2 \) is odd.

For each two-qubit state, the lower and upper bounds in (50) coincide and (50) reduces to

\[
\max_{A_1, B_1, B_2 \in L_2} |\text{tr}[\rho_{2 \times 2} B_{\text{CHSH}}(A_1, A_2; B_1, B_2)]| = 2 \sqrt{\lambda_{\rho_{2 \times 2}} + \tilde{\lambda}_{\rho_{2 \times 2}}},
\]

(51)

i. e. to the precise two-qubit result found by Horodecki in [6].

As we prove in Section 4, for the two-qudit GHZ state, the upper bound (50) is also attained and gives the precise value for the maximum of the CHSH expectation (51) in this state.

4 The two-qudit GHZ state

Let us specify the upper bound (50) for the two-qudit GHZ state

\[
\rho_{\text{GHZ},d} = \frac{1}{d} \sum_{j,k=1,\ldots,d} |j\rangle \langle k| \otimes |j\rangle \langle k|.
\]

(52)

For this state, the correlation matrix \( T_{\rho_{\text{GHZ},d}} \) is hermitian. Calculating its elements due to relation (35) and expressions (3), (4)–(6), we come for this matrix to the diagonal block form

\[
\begin{pmatrix}
T^{(s)} & 0 & 0 \\
0 & T^{(as)} & 0 \\
0 & 0 & T^{(d)}
\end{pmatrix}
\]

(53)
where

(i) \( T^{(s)} \) is the \( \frac{d(d-1)}{2} \times \frac{d(d-1)}{2} \) matrix with elements

\[
\text{tr}[\rho_{ghz,d}\{\Lambda^{(s)}_{jk} \otimes \Lambda^{(s)}_{j_1k_1}\}], \quad j, j_1, k, k_1 = 1, \ldots, \frac{d(d-1)}{2},
\]

which are equal to \( \frac{\delta}{d} \) on the diagonal and to zero, otherwise;

(ii) \( T^{(as)} \) is the \( \frac{d(d-1)}{2} \times \frac{d(d-1)}{2} \) matrix with elements

\[
\text{tr}[\rho_{ghz,d}\{\Lambda^{(as)}_{jk} \otimes \Lambda^{(as)}_{j_1k_1}\}], \quad j, j_1, k, k_1 = 1, \ldots, \frac{d(d-1)}{2},
\]

which are equal to \( (\frac{-2}{d^2}) \) on the diagonal and to 0, otherwise;

(iii) \( T^{(d)} \) is the \( (d-1) \times (d-1) \) matrix with elements

\[
\text{tr}[\rho_{ghz,d}\{\Lambda^{(d)}_{l} \otimes \Lambda^{(d)}_{l_1}\}], \quad l, l_1 = 1, \ldots, d-1,
\]

which are equal to \( \frac{\delta}{d} \) on the diagonal and to zero, otherwise.

Thus, for the two-qudit GHZ state \([52]\), the positive hermitian matrix

\[
T^*_{\rho_{ghz,d}} T_{\rho_{ghz,d}} = T^2_{\rho_{ghz,d}} = \frac{4}{d^2} \mathbb{I}_{d^2-1},
\]

and each vector \( n \in \mathbb{R}^{d^2-1} \) is an eigenvector of \( T^2_{\rho_{ghz,d}} \) with eigenvalue \( \frac{4}{d^2} \). From \([57]\) it follows that, for the GHZ state, the eigenvalues in \([50]\) are given by

\[
\lambda_{\rho_{ghz,d}} = \tilde{\lambda}_{\rho_{ghz,d}} = \frac{4}{d^2},
\]

so that, for the GHZ state, the general upper bound in \([50]\) reduces to

\[
\max_{A_i, B_k \in \mathcal{L}_d} \left| \text{tr}[\rho_{ghz,d} B_{\text{chsh}}(A_1, A_2; B_1, B_2)] \right| \leq 2 l_d^4 \sqrt{2},
\]

where \( l_d = d \) if a dimension \( d \geq 2 \) is even and \( l_d = \sqrt{\frac{d-1}{d}} \) if a dimension \( d \geq 2 \) is odd. This proves the following statement.

**Proposition 2** For the two-qudit GHZ state \([62]\), the new upper bound introduced in Theorem 1 is equal to \( 2 l_d^4 \sqrt{2} \) and, if a qudit dimension \( d \geq 2 \) is odd, this upper bound is better than the general upper bound \( 2 \sqrt{2} \) of Tsirelson \([3, 4]\).

Furthermore, let us prove that, for the GHZ state, the upper bound \([50]\) is attained.

If \( d = 2 \), then the two-qubit GHZ state constitutes the Bell state and the upper bound \([59]\) is attained.

Consider an arbitrary \( d > 2 \). From \([53]-[56]\) it follows that each vector \( r \in \mathbb{R}_d \) is decomposed via \( r = r^{(+) +} + r^{(-)} \), where \( \langle r^{(+)}, r^{(-)} \rangle = 0 \) and

\[
T_{\rho_{ghz,d}} r^{(\pm)} = \pm \frac{2}{d} r^{(\pm)}.
\]

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Let $X$ be a traceless qudit observable with $d$ mutually orthogonal unit eigenvectors given by the unit vectors in the computational basis \{\ket{j}, j = 1, \ldots, d\} of $\mathbb{C}^d$ and eigenvalues \{\pm 1\} – if a dimension $d > 2$ is even and \{0, \pm 1\} – if a dimension $d > 2$ is odd.

Due to the structure (4)–(5) of traceless qudit operators $\Lambda_{jk}^{(s)}$, $\Lambda_{jk}^{(as)}$, under representation (19), to this observable $X$ there corresponds a vector $r_X \in \mathbb{R}^d$, for which $r_X^r = 0$, so that $r_X = r_X^+$. For this vector: (i) $\|r_X^+ \cdot \Lambda_0\|_0 = \sqrt{2/d}$ by (17) and (ii) $\|r_X^+\| = l_d$ – as specified in lines after (24). Moreover, for $d > 2$, we can always find at least two such observables $X_1$ and $X_2$, for which $r_{X_1}^+ \neq -r_{X_2}^+$.

Taking all this into account for the maximum in the second line of (46), we have:

$$\sqrt{2d} \max_{r_1, r_2 \in \mathbb{R}^d} \left[ \frac{\|T_{p_{d \times d} r_1}^0\|^4}{\|T_{p_{d \times d} r_2}^0\|^2} + \frac{\|T_{p_{d \times d} r_2}^0\|^2}{\|T_{p_{d \times d} r_2}^0\|^2} \right] \geq \sqrt{2d} \left( \frac{4}{d^2} \frac{\|r_{X_1}^+\|^4}{\|r_{X_1}^+ \cdot \Lambda_0\|^2} + \frac{4}{d^2} \frac{\|r_{X_2}^+\|^4}{\|r_{X_2}^+ \cdot \Lambda_0\|^2} \right) = 2l_d^2 \sqrt{2}. $$

Therefore, Eqs. (60), (61) imply

$$\max_{A_i, B_k \in L_d} \left| \tr[\rho_{ghz,d} B_{chsh}(A_1, A_2; B_1, B_2)] \right| \geq 2l_d^2 \sqrt{2}. $$

Comparing (59) and (62), we come to the following new result.

**Theorem 2** For the two-qudit GHZ state $\rho_{ghz,d}$ with an arbitrary $d \geq 2$, the upper bound in Theorem 1 is attained for each $d \geq 2$ and specifies the maximal value for the CHSH expectation (31) in this state:

$$\max_{A_i, B_k \in L_d} \left| \tr[\rho_{ghz,d} B_{chsh}(A_1, A_2; B_1, B_2)] \right| = 2l_d^2 \sqrt{2}. $$

Here, $l_d^2 = 1$ if a qudit dimension $d \geq 2$ is even and $l_d^2 = \frac{d-1}{d}$ if a qudit dimension $d \geq 2$ is odd.

This result for the maximal value of the CHSH expectation in the GHZ state can be also derived if to substitute the correlation matrix (53) directly into maximum (38).

**5 Conclusions**

In the present paper, we have formulated and proved the properties (Proposition 1) of the generalized Gell–Mann representation for traceless qudit observables and studied via this representation violation of the CHSH inequality by a two-qudit state ($d \geq 2$).
For the maximal value

$$\max_{A_i, B_k \in \mathcal{L}_d} | \text{tr}[\rho_{d \times d} B_{\text{chsh}}(A_1, A_2; B_1, B_2)] |$$  \hspace{1cm} (64)$$

of the CHSH expectation in a two-qudit state $\rho_{d \times d}$ with an arbitrary qudit dimension $d \geq 2$, we have derived the precise expression (46) for the maximum (64) in terms of the correlation matrix of this state – which explicitly leads to the general upper bound of Tsirelson [3, 4], and due to this new expression – two new bounds, lower and upper, formulated via the eigenvalues of the correlation matrix of a two-qudit state $\rho_{d \times d}$.

We have not yet been able to specify a class of two-qudit states for which the new upper bound improves the general upper bound of Tsirelson [3, 4]. However, this is the case:

(i) for each two-qubit state, where the new lower bound and the new upper bound in Theorem 1 coincide and reduce to the precise value of (64) found by Horodecki [6];

(ii) for the two-qudit GHZ state (52) with an arbitrary odd $d \geq 2$, where the new upper bound is less (Proposition 2) than the upper bound of Tsirelson [3, 4].

Moreover, for the GHZ state (52), we have explicitly found its correlation matrix and proved (Theorem 2) that, for the two-qudit GHZ state with an arbitrary qudit dimension $d \geq 2$, the new upper bound is attained (Theorem 2) and this specifies the following new result: the maximal violation of the CHSH inequality by the two-qudit GHZ state is equal to $\sqrt{2}$ if a qudit dimension $d \geq 2$ is even and to $\frac{d-1}{d} \sqrt{2}$ if a qudit dimension $d \geq 2$ is odd.

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6 Appendix A

Consider the proof of Lemma 1. The operator norm of a qudit observable $n \cdot \Lambda$ is given by

$$\|n \cdot \Lambda\|_0 := \sup_{\|\psi\| = 1, \psi \in \mathbb{C}^d} | \langle \psi, (n \cdot \Lambda) \psi \rangle | = \sup_{\|\psi\| = 1, \psi \in \mathbb{C}^d} | \text{tr}[(n \cdot \Lambda) |\psi\rangle \langle \psi|] |$$  \hspace{1cm} (A1)$$

For a pure state $|\psi\rangle \langle \psi|$, the normalized version of decomposition (1) reads

$$|\psi\rangle \langle \psi| = \frac{1}{d} I_{\mathbb{C}^d} + \frac{d-1}{2d} (r_{\psi} \cdot \Lambda), \quad r_{\psi}^{(j)} = \sqrt{\frac{d}{2(d-1)}} \langle \psi, \Lambda_j \psi \rangle$$  \hspace{1cm} (A2)$$

where $r_{\psi} \in \mathbb{R}^{d^2-1}$. Since $\text{tr}[\Lambda_j] = 0$, it follows from (A2) and (2) that

$$1 = \frac{1}{d} + \frac{d-1}{d} \|r_{\psi}\|^2 \ \Leftrightarrow \ \|r_{\psi}\| = 1, \ \|\psi\| = 1, \ \psi \in \mathbb{C}^d.$$  \hspace{1cm} (A3)$$
Substituting (A2) into (A1) and taking into account (2), (A3), we have
\[ \| n \cdot \Lambda \|_0 = \sqrt{\frac{2(d-1)}{d}} \left( \sup_{\| \psi \| = 1, \psi \in \mathbb{C}^d} | \langle n, r \psi \rangle | \right) \leq \sqrt{\frac{2(d-1)}{d}} \| n \|. \] (A4)

This proves the upper bound in (9). To prove the lower bound and the last upper bound in (9), we use (8) and relations
\[ (1 + \delta_d) \| n \cdot \Lambda \|_0^2 \leq \text{tr}[(n \cdot \Lambda)^2] = 2 \| n \|^2 \leq d \| n \cdot \Lambda \|_0^2, \] (A5)
which imply
\[ \frac{2}{d} \leq \frac{\| n \cdot \Lambda \|_0^2}{\| n \|^2} \leq \frac{2}{1 + \delta_d}. \] (A6)

Eqs. (A4), (A6) prove the statement of Lemma 1.

7 Appendix B

Consider the proof of Theorem 1. According to (27) and (25)
\[ \sqrt{\frac{2}{d}} \| T_{\rho_{d \times d}} n \| \leq l_d, \quad \forall n \in \mathbb{R}^{d^2-1}. \] (B1)

Also, by the upper bound in (9)
\[ \| T_{\rho_{d \times d}} n \| \geq \sqrt{\frac{d}{2(d-1)}}, \quad \forall n \in \mathbb{R}^{d^2-1}. \] (B2)

Relations (B1), (B2) imply
\[ \sqrt{\frac{d}{2(d-1)}} \leq \frac{\| T_{\rho_{d \times d}} n \|}{\| T_{\rho_{d \times d}} n \cdot \Lambda \|_0} \leq l_d \sqrt{\frac{d}{2}} \] (B3)

Substituting this into the maximum in the second line of (40), we derive
\[ \frac{d}{\sqrt{d-1}} \max_{r_1, r_2 \in \mathbb{R}_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2} \] (B4)
\[ \leq \sqrt{2d} \max_{r_1, r_2 \in \mathbb{R}_d} \sqrt{\frac{\| T_{\rho_{d \times d}} r_1 \|_0^4 + \| T_{\rho_{d \times d}} r_2 \|_0^4}{\| T_{\rho_{d \times d}} r_1 \cdot \Lambda \|_0^2 + \| T_{\rho_{d \times d}} r_2 \cdot \Lambda \|_0^2}} \] (B5)
\[ \leq l_d d \max_{r_1, r_2 \in \mathbb{R}_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2} \]
Taking further into account that, in view of (24), (26), \( \mathcal{R}_d \) is a subset of the ball of radius \( l_d \) and also contains the ball of radius \( \frac{1}{\sqrt{d-1}} \), we have

\[
\max_{r_1, r_2 \in \mathcal{R}_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2} \quad (B5)
\]

\[
\leq \max_{\|r_1\|, \|r_2\| \leq l_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2}
\]

\[
= \max_{l.i., \|r_1\|, \|r_2\| = l_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2}
\]

and

\[
\max_{r_1, r_2 \in \mathcal{R}_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2} \quad (B6)
\]

\[
\geq \max_{\|r_1\|, \|r_2\| \leq \frac{1}{\sqrt{d-1}}} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2}
\]

\[
= \max_{l.i., \|r_1\|, \|r_2\| = \frac{1}{\sqrt{d-1}}} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2}
\]

where abbreviation "l.i." in the third lines of (B5), (B6) means linear independent and appears since the transition from maximums in the second lines in (B5), (B6) to the maximums in the third lines takes already into account maximums over vectors \( r_1, r_2 \) along the same ray inside the ball, that is, linear dependent \( r_1, r_2 \).

Therefore, from (B4)–(B6) it follows

\[
\frac{d}{\sqrt{d-1}} \max_{l.i., \|r_1\|, \|r_2\| = \frac{1}{\sqrt{d-1}}} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2} \quad (B7)
\]

\[
\leq \sqrt{2d} \max_{r_1, r_2 \in \mathcal{R}_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^4 + \| T_{\rho_{d \times d}} r_2 \|^4} \quad \| T_{\rho_{d \times d}} \cdot \Lambda \|^2_0 \quad \| T_{\rho_{d \times d}} \cdot \Lambda \|^2_0
\]

\[
\leq l_d \max_{l.i., \|r_1\|, \|r_2\| = l_d} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2}.
\]

Note also that, for each radius \( R_0 \) of the sphere in \( \mathbb{R}^{d^2-1} \),

\[
\max_{l.i., \|r_1\|, \|r_2\| = R_0} \sqrt{\| T_{\rho_{d \times d}} r_1 \|^2 + \| T_{\rho_{d \times d}} r_2 \|^2} \quad (B8)
\]

\[
= R_0 \sqrt{\lambda_{\rho_{d \times d}} + \tilde{\lambda}_{\rho_{d \times d}}},
\]

where \( \lambda_{\rho_{d \times d}} \geq \tilde{\lambda}_{\rho_{d \times d}} \geq 0 \) are two greater eigenvalues, corresponding to two linear independent eigenvectors of the positive hermitian matrix \( T_{\rho_{d \times d}}^* \cdot T_{\rho_{d \times d}} \).
Substituting (66) into (66), we derive

\[
\frac{d}{d-1} \sqrt{\lambda_{p_{d \times d}} + \tilde{\lambda}_{p_{d \times d}}} \tag{B9}
\]

\[
\leq \sqrt{2d} \max_{r_1,r_2 \in \mathbb{R}^d} \sqrt{\frac{\| T_{p_{d \times d} r_1} \|_2^4 + \| T_{p_{d \times d} r_2} \|_2^4}{\| T_{p_{d \times d} r_1} \lambda \|_0^2 + \| T_{p_{d \times d} r_2} \lambda \|_0^2}}
\]

\[
\leq \frac{l_d^2}{d} \sqrt{\lambda_{p_{d \times d}} + \tilde{\lambda}_{p_{d \times d}}}
\]

In view of (66), this proves the statement of Theorem 1.

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