Simple conditions constraining the set of quantum correlations

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The characterization of the set of quantum correlations in Bell scenarios is a problem of paramount importance for both the foundations of quantum mechanics and quantum information processing in the device-independent scenario. We provide here simple and general analytical conditions that are necessary for an arbitrary bipartite behaviour to be quantum. Although the conditions are not sufficient, we illustrate the strength and non-triviality of these conditions with a few examples. Moreover, we provide several applications of this result: we prove the separation of the quantum set from extremal nonlocal no-signaling behaviours in several general scenarios, we provide a systematic construction to obtain Tsirelson bounds for arbitrary Bell inequalities and we construct a Bell expression whose maximal quantum value is attained by a maximally entangled state of qutrits.

Bell’s theorem shows that the correlations exhibited by quantum mechanical systems go beyond what is achievable by any local realistic theory (i.e. any local hidden variable model) [1]. This result has deep implications and still spurs several subfields of research [2]. On the one hand, from a foundational perspective, it has been questioned what physical principle in nature could then be responsible for giving rise to precisely the particular set of correlations allowed by quantum mechanics. Since it has been shown that this set is strictly smaller that what could be achieved by just imposing the no-signaling principle (i.e. the impossibility of super-luminal or instantaneous propagation of information) [3, 4], several works have considered more restrictive physically-motivated axioms [5–7]. Although these approaches rule out several subsets of no-signaling correlations, no definite answer has yet been found as there still exist supra-quantum correlations compatible with these principles [8]. On the other hand, from a more practical point of view and in the context of quantum information theory, it has been realized that quantum nonlocality can be regarded as a resource for device-independent quantum information processing (DIQIP). The tasks that can be carried out in this way include key distribution for cryptography [9], randomness generation [10] and dimensionality certification (see e.g. [11, 12]).

In order to understand which physical principles constrain the set of quantum correlations and to elucidate what are the ultimate limitations behind DIQIP protocols, a fundamental question arises: can an efficient expression whose maximal quantum value is attained by a maximally entangled state of qutrits.

Simple conditions constraining the set of quantum correlations. These could be used to exclude some general subsets of no-signaling correlations from the quantum set based on their analytical properties or to bound the maximal efficiency a particular DIQIP task can attain provided that any implementation we can think of must ultimately be quantum. The aim of this Letter is to fill this gap by providing simple general analytical conditions any quantum behaviour should satisfy. Although these conditions emerge from the first step of the NPA hierarchy and, therefore, there exist supra-quantum correlations that do not violate them, I will provide examples showing their strength and non-triviality. It is the author’s hope that these conditions will be of use in the field of quantum nonlocality and DIQIP. To support this claim, I will further provide several applications of this result: a proof of the separation between the quantum set and extremal nonlocal no-signaling correlations (a question recently raised in [14]), a systematic way to obtain quantum bounds on arbitrary Bell inequalities (generalizing the recent result [15]) and the possibility to do robust self-testing of bipartite maximally entangled states by building Bell inequalities that are maximally violated by them.

Framework and main result. We will consider the standard bipartite Bell scenario [2] in which two parties $A$ and $B$ that could have interacted in the past remain now uncommunicated. Party $A$ ($B$) can freely choose questions from a finite alphabet $\mathcal{X} = \{1, 2, \ldots, m_A\}$ ($\mathcal{Y} = \{1, 2, \ldots, m_B\}$). Given any of these inputs $x \in \mathcal{X}$ and $y \in \mathcal{Y}$, each party can obtain an outcome $a \in A = \{1, 2, \ldots, d_A\}$ and $b \in B = \{1, 2, \ldots, d_B\}$, where the output alphabets are also finite. For every fixed choice of size of the alphabets, we will denote this scenario by $(m_A m_B d_A d_B)$. The central object here, referred to as behaviour, is the joint conditional probability distribution of obtaining the outputs $(a,b)$ given the choice of inputs $(x,y)$, $P(ab|xy)$ (for which we will use the shorthand $P$). This list of $d_A d_B m_A m_B$ numbers must fulfill $P(ab|xy) \geq 0 \forall a, b, x, y$ and $\sum_{a,b} P(ab|xy) = 1 \forall x, y$. Moreover, since communi-
cation among the parties is not possible during the choice of input and recording of the output, the marginal of each party must be independent of the other's action, $P(a|x) = \sum_y P(ab|xy) = \sum_y P(ab|yx)$ for all $x, y \neq y'$ and $P(b|y) = \sum_a P(ab|xy) = \sum_a P(ab|x'y) \forall b, y, x \neq x'$. The set of all behaviours satisfying these no-signalling conditions will be denoted by $\mathcal{NS}$. Particular elements of this set are the $d^m_A \times d^m_B$ different local deterministic behaviours (LDBs) $D_i(ab|xy) = \delta_{a, f_i(x)} \delta_{b, g_i(y)}$ in which for every party a unique output occurs with probability 1 for every choice of input. The convex hull of these behaviours gives rise to the local set $\mathcal{L}$ [16]. On the other hand, the quantum set $\mathcal{Q}$ is given by all behaviours that can be obtained by performing measurements on bipartite quantum states of unrestricted dimension $\rho_{AB}$, i.e. $P(ab|xy) = \text{tr}(\rho_{AB} \Pi^a_x \otimes \Pi^b_y)$ for some projectors fulfilling $\sum_a \Pi^a_x$ and $\sum_b \Pi^b_y$ being equal to the identity in each party's Hilbert space $\forall x, y$. The crucial observation mentioned in the introduction is that $\mathcal{L} \subseteq \mathcal{Q} \subseteq \mathcal{NS}$. Although it is clear that $\mathcal{Q}$ is a convex set, one can see that it is in general very hard to decide from the definition whether a given behaviour is in $\mathcal{Q}$ or not. On the contrary, $\mathcal{L}$ and $\mathcal{NS}$ are both convex polytopes with vertices given by the LDBs in the first case, to which we have to add some non-local vertices in the second case. Following the standard notation, we will refer to these extremal non-local behaviours as Popescu-Rohrlich (PR) boxes.

In order to present our results, we will use some further notation. We will arrange every $P \in \mathcal{NS}$ to form the $m_A d_A \times m_B d_B = n_A \times n_B$ real matrix $P = \sum_{abxy} P(ab|xy)|xa\rangle\langle yb|$, where in the standard notation of quantum mechanics $|xa\rangle = |x\rangle \otimes |a\rangle$ and $\{|x\rangle\}$ denotes the computational basis of $\mathbb{R}^{m_A}$ and similarly for the other alphabet elements. Thus, $P$ can be partitioned as a block matrix with blocks

$$P_{xy} = \begin{pmatrix} P(1|1|xy) & \cdots & P(1|d_B|xy) \\ \vdots & \ddots & \vdots \\ P(d_A|1|xy) & \cdots & P(d_A|d_B|xy) \end{pmatrix} \in \mathbb{R}^{d_A \times d_B}.$$ 

Normalisation imposes that the entries in each block add up to one while no-signaling that the sum of the elements in the same row (column) for blocks in the same row (column) is equal. We will consider different matrix norms. Following the Schatten p-norm notation, $\| \cdot \|_p$ will be the trace norm (i.e. the sum of all singular values) while $\| \cdot \|_\infty$ the spectral norm (i.e. the maximal singular value). We are now in the position to state our main result.

**Theorem 1.** In every $(m_A m_B d_A d_B)$ scenario, if $P \in \mathcal{Q}$ then $\|P\|_1 \leq \sqrt{m_A m_B}$. 

We will actually prove the following stronger result: for every $P \in \mathcal{Q}$ it must hold that

$$\langle P, G \rangle = \text{tr}(PG^T) = \sum_{abxy} P(ab|xy)G(ab|xy) \leq \|G\|_\infty \sqrt{m_A m_B} \quad \forall G \in \mathbb{R}^{n_A \times n_B}. \quad (1)$$

The relevance of this result will be discussed later on. For the moment, let us simply point out that Theorem 1 follows from it by noticing that $\|P\|_1 = \max_O \text{tr}(PO)$ where the maximization is over all isometries [17]. As mentioned in the introduction, to prove inequality (1) we will use the first step of the NPA hierarchy, $Q^1$. Since $Q \subset Q^1$, it suffices to prove the inequality $\forall P \in Q^1$, which we do in the Appendix.

One of the appealing properties of Theorem 1 and inequality (1) is that they have a very compact form. Before discussing their strength and applications, it should be stressed that the reasoning used in their proof can be applied to obtain other stronger but more complicated conditions. As we will see later this line of thought can also be applied in the correlation picture. Let us denote by $M$ the matrix constructed using the same prescription as $P$ but with entries given by $M(ab|xy) = P(ab|xy) - P(a|x)P(b|y)$. Using similar ideas as in the proof of Theorem 1 (see Appendix), we arrive at that for any choice of $G$, $\langle M, G \rangle \leq \|G\|_\infty \sqrt{m_A m_B} - \frac{\|G\|_\infty}{2} \sum_{ab} P(ab)^2 - \frac{\|G\|_\infty}{2} \sum_{ab} P(b|y)^2$ should hold $\forall P \in Q$ and, hence

**Theorem 2.** In every $(m_A m_B d_A d_B)$ scenario, if $P \in \mathcal{Q}$ then

$$\|M\|_1 \leq \sqrt{m_A m_B} \left( 1 - \sum_{abxy} \frac{P(ab)^2}{2m_A} - \sum_{abxy} \frac{P(b|y)^2}{2m_B} \right).$$

Notice that our conditions have been deduced from the definition of the first step of the NPA hierarchy, $Q^1$. Obviously then, the best we can expect from them is to separate this set from its complement in $\mathcal{NS}$. Therefore, since $\mathcal{Q} \subset Q^1$, it is clear that there exist supra-quantum behaviours satisfying the conditions of Theorems 1 and 2 (i.e. they are necessary for a behaviour to be in $\mathcal{Q}$ but not sufficient). In the simplest setting (2222), $Q^1$ can be characterized by a simple inequality [13]. We have performed numerical explorations in this scenario that show that the gap between $Q^1$ and the behaviours satisfying our conditions is small. Theorem 2 only provides a slightly better approximation of $Q^1$ than Theorem 1. A more detailed example can be found in Figure 1. To my knowledge, the only previous instance of analytical means to constrain $Q$ is given by the results of [18] (which emerge from $Q^1$ as well). However, the application of these techniques is not completely straightforward as they rely on some choice of data processing. Still, the inequality emerging from this approach reproduces $Q^1$ in the (2222) scenario. Notwithstanding, Figure 1 shows that our conditions give a much tighter restriction already in the (3322) example considered in [18]. This is also apparent in the (2233) case, where the results presented in [18] fail to completely reproduce $Q^1$ for the isotropic behaviours obtained by mixtures of a fully random box and the PR box $F_{PR}(2, 3)$ (see Eq. (2) below).
On the contrary, Theorems 1 and 2 are tight in this case. To show further the usefulness of these results, in the remaining we provide several applications of them.

**Nontriviality of the conditions and nonquantumness of extremal no-signaling behaviours.** The previous examples already give a good idea of the strength of the conditions derived here. To analyze in full generality their non-triviality, notice that, due to the convexity of the trace norm, $\|P\|$ must attain its maximum value in NS at the vertices of the NS polytope. Hence, the ideal situation would be that the LDBs achieve the maximal possible value ($\sqrt{mAmB}$) and that all PR boxes violate this bound. Actually, it has been recently shown in [14] that all PR boxes (including the multipartite case) are not in Q. It was left as an open question there whether there exists a separation between them and Q since the closest to these behaviours the more efficient certain applications of DIQIP can be [14]. In the following we show that all LDBs attain the $\sqrt{mAmB}$ bound and that all PR boxes in (22dAdb) and (mm22) scenarios violate the bound. Thus, besides showing that our condition is in general not trivial, we further provide a simple proof in these cases of the result of [14]. Moreover, we show that there actually exists a separation between these PR boxes and Q, answering in these scenarios the question raised therein.

**Proposition 3.** In every (mAmBdAdB) scenario, if $P \in \mathcal{L}$ then $\|P\| \leq \sqrt{mAmB}$, with equality for LDBs.

The proof of this proposition is given in the Appendix. That the inequality is fulfilled in L is obvious from Theorem 1. The important observation here is that all LDBs attain the bound, hence showing that it cannot be improved. Let us consider now the (22dAdb) scenario and let $d = \min(d_A, d_B)$. The PR boxes in this case are given by [33]

$$P_{PR}(2, d) = \frac{1}{d} \left( \begin{array}{ccc} 1_d & 1_d & \ldots & 1_d \\ 1_d & 0_d & \ldots & 0_d \\ \vdots & \ddots & \ddots & \vdots \\ 0_d & \ldots & 0_d & 1_d \end{array} \right), \quad A_d = \left( \begin{array}{c} 0 \\ \vdots \\ 0 \end{array} \right).$$

up to relabelings of the inputs and the outputs [19]. Since these transformations amount to certain permutations of the rows or columns of P that leave the trace norm invariant, it suffices to compute it for the matrix given in Eq. (2). Using the pinching inequality [20, 21], we obtain that

$$\|P_{PR}(2, d)\|_1 \geq \frac{1}{d} \left( \|1_d\|_1 + \|A_d\|_1 \right) = 2.$$

The conditions under which equality is attained in the pinching inequality are given in Theorem 8.7 of [21] and it is easily checked that they are not met in this case. Hence, we obtain that $\|P_{PR}(2, d)\|_1 > 2$, which amounts to the non-quantumness of these PR boxes by Theorem 1. Moreover, by a more refined use of the pinching inequality, we show in the Appendix that $\|P_{PR}(2, d)\|_1 \geq \sqrt{5} - 2$. We therefore obtain the following separation theorem.

**Theorem 4.** In every (22dAdb) scenario, it holds $\forall P \in Q$ that $\|P_{PR}(2, d) - P\|_1 \geq \|P_{PR}(2, d)\|_1 - \|P\|_1 \geq \sqrt{5} - 2$.

It might be interesting to note that $\|P_{PR}(2, d)\|_1 \leq 2 + \sqrt{2}$, which we also prove in the Appendix. Numerics suggest that the above estimates can be improved to $1 + \sqrt{2} = \|P_{PR}(2, d)\|_1 \leq \|P_{PR}(2, d)\|_1 < \lim_{d \to \infty} \|P_{PR}(2, d)\|_1 \simeq 2.55$, that would change the bound in Theorem 4 to $2 - 1$. Let us move now to the (mm22) scenario. The corresponding PR boxes have all been determined in [22] (see Table II therein). We denote an arbitrary one of them by $P_{PR}(m, 2)$. One sees that (up to relabelings) these matrices always have the following structure: they have a 4 x 4 block in the diagonal given by $P_{PR}(2, 2)$ followed by $m - 2 \times 2$ blocks in the diagonal, which are either $1_2$ or $A_2$ or $diag(1, 0)$. Since the latter blocks all have unit trace norm, it follows again by the pinching inequality that $\|P_{PR}(m, 2)\|_1 \geq \|P_{PR}(2, 2)\|_1 + m - 2 = m + \sqrt{2} - 1$.

**Theorem 5.** In every (mm22) scenario, it holds $\forall P \in Q$ that $\|P_{PR}(m, 2) - P\|_1 \geq \|P_{PR}(m, 2)\|_1 - \|P\|_1 \geq \sqrt{2} - 1$.

It might be interesting to mention as well that $\|P_{PR}(m, 2)\|_1 \leq m\sqrt{m}$ (see Appendix).
Tsirelson bounds. The familiar reader will have already noticed that the left-hand-side of inequality (1) defines an arbitrary Bell expression. These are any linear combination of the elements \( P(ab|xy) \). Since \( \mathcal{L}, \mathcal{Q} \) and \( \mathcal{NS} \) are compact convex sets, there always exist such expressions separating, i.e. \( \langle P, G \rangle \leq G_{\mathcal{L}}, G_{\mathcal{Q}}, G_{\mathcal{NS}} \) depending on whether \( P \in \mathcal{L}, \mathcal{Q}, \mathcal{NS} \) with \( G_{\mathcal{L}} \leq G_{\mathcal{Q}} \leq G_{\mathcal{NS}} \). The most characteristic one is the CHSH inequality (see below) in the (2222) scenario for which \( G_{\mathcal{L}} = 2 [23], G_{\mathcal{Q}} = 2\sqrt{2} [24] \) and \( G_{\mathcal{NS}} = 4 [4] \). While to determine the optimal value of \( G_{\mathcal{L}} \) and \( G_{\mathcal{NS}} \) it suffices to check over the corresponding vertices, to determine the optimal value of \( G_{\mathcal{Q}} \), known as Tsirelson bounds, is a less straightforward task [34]. However, this is very relevant to identify optimal DQI/QP performances in the context of quantum games [2]. Thus, a remarkable feature of inequality (1) is that it provides a systematic way to construct quantum upper bounds to arbitrary Bell inequalities. Actually, our result resembles very much that recently found in [15], with the difference that the latter only holds for the particular class of Bell inequalities based on correlators. Later on, we will see that this result can also be deduced using our ideas and we will put it in context. To give a hint of the usefulness of inequality (1), we will show now that it allows to obtain Tsirelson’s bound for the CHSH inequality. This can be expressed by a matrix \( G_{CHSH} \) with blocks given by \( G_{11} = G_{12} = G_{21} = -G_{22} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \). It turns out that \( \|G_{CHSH}\|_{\infty} = 2 \) and, hence, we obtain the trivial bound 4. Nevertheless, it must be stressed that, given that behaviours in \( \mathcal{NS} \) must fulfill several different constraints, the same Bell inequality can be expressed with many different choices of the matrix \( G \). Thus, if we take

\[
G'_{CHSH} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} + \frac{1}{2\sqrt{2}} G_{CHSH},
\]

it holds that \( \|G'_{CHSH}\|_{\infty} = 1 \). We have then that \( \forall P \in \mathcal{Q}, \langle P, G'_{CHSH} \rangle = 1 + \langle P, G_{CHSH} \rangle / (2\sqrt{2}) \leq 2 \) and, hence, \( \langle P, G_{CHSH} \rangle \leq 2\sqrt{2} \).

Since the CHSH Tsirelson bound is achievable by a quantum behaviour arising from certain measurements on a maximally entangled two-qubit state and \( G'_{CHSH} \) is orthogonal, this also shows that for this behaviour \( \|P\|_1 = 2 \), achieving the bound of Theorem 1. It is a natural question to ask which other behaviours in \( \mathcal{Q} \setminus \mathcal{L} \) can attain it. On the analogy of this example, one could conjecture that this could be the case for behaviours maximally violating some facet Bell inequality. However, we computed \( \|P\|_1 \) for the quantum behaviours yielding the largest known value for several two-outcome Bell inequalities given in [25] but, in general, the bound of Theorem 1 is not attained. Interestingly, when this occurs, the behaviour arises from a maximally entangled state of qubits. This seems to extend for scenarios with more outcomes. In particular, in (2233) the quantum behaviour maximally violating the CGLMP inequality [26] was given in [27] as proved in [13]. However, for it we find that \( \|P\|_1 \approx 1.98 \), while the maximal value \( \|P\|_1 = 2 \) is attained for the behaviour that yields the maximal CGLMP value from measurements on a maximally entangled two-qutrit state [26, 27], despite its CGLMP value being lower. As we show in the Appendix, from this it is immediate to construct a Bell inequality, \( G(\Phi_x^+) \), whose maximal value in \( \mathcal{Q} \) (which is strictly larger than that in \( \mathcal{L} \)) is attained then by a two-qutrit maximally entangled state. This might be of relevance in the context of self-testing [28] if it turned out that this behaviour is the only one maximizing \( G(\Phi_x^+) \) in \( \mathcal{Q} \). Self-testing arises when a certain behaviour is the unique to attain a particular Bell value. For instance, \( \langle P, G_{CHSH} \rangle = 2\sqrt{2} \) is only possible for a behaviour coming from an effective maximally entangled two-qubit state [29]. This allows to check the performance of a quantum set-up without trusting any of the devices, particularly when it can be made robust [30, 31] (i.e. when it can be guaranteed that if the Bell value is close to maximal, then the fidelity is close too to the target state). Using the techniques of [31] with the Bell inequality \( G(\Phi_x^+) \), it should be possible to check whether robust self-testing of a a two-qutrit maximally entangled state is possible in this way.

Correlation scenarios. If we restrict ourselves to two-outcome scenarios (\( d_A = d_B = 2 \)) and taking \( a, b \in \{-1, 1\} \), all behaviours in \( \mathcal{NS} \) can be alternatively characterized by the correlators \( \langle A_x B_y \rangle = \sum_{ab} a b P(ab|xy) \) and the marginal expectations \( \langle A_x \rangle = \sum_a a P(a|x) \) and \( \langle B_y \rangle = \sum_b b P(b|y) \). As mentioned before, it has been shown in [15] that for the particular class of correlator Bell inequalities \( \sum_{xy} G_{xy} \langle A_x B_y \rangle \leq \|G\|_{\infty} \sqrt{m_A m_B} \) must hold \( \forall P \in \mathcal{Q} \) and every real \( m_A \times m_B \) matrix \( G \). In the Appendix we show that this result can also be proved using similar techniques as in Theorems 1 and 2 [32]. This does not only provide an alternative proof of this fact but it also shows that this bound cannot give stronger constraints than \( Q^1 \). Moreover, as in Theorems 1 and 2 this leads to the following condition

\[
\|C\|_1 \leq \sqrt{m_A m_B} \quad \forall P \in \mathcal{Q},
\]
\[ \frac{\|G\|}{2} = \sqrt{\frac{m_B}{m_A}} \sum_x (A_x)^2 - \frac{\|G\|}{2} \sqrt{\frac{m_A}{m_B}} \sum_y (B_y)^2 \forall P \in Q, \]

which particularly implies

\[ \|C'\| \leq \sqrt{m_A m_B} \left( 1 - \frac{1}{2m_A} \sum_x (A_x)^2 - \frac{1}{2m_B} \sum_y (B_y)^2 \right), \quad (4) \]

where \( C' \) has now entries \( C'_{xy} = \langle A_x B_y \rangle - \langle A_x \rangle \langle B_y \rangle \).

**Conclusions.** We have shown that the first step of the NPA hierarchy allows to obtain simple analytical conditions constraining the set of quantum behaviours in general bipartite Bell scenarios, whose strength and non-triviality have been illustrated. Since not all problems in quantum nonlocality and DIQIP can be addressed numerically, we expect these conditions to be of utility, filling the hitherto lack of such general tools. In fact, we have applied these results to show the separation of the quantum set and PR boxes in several scenarios and, generalizing the results of [15], we have provided a systematic construction of quantum bounds for arbitrary Bell inequalities. Moreover, since it seems that outside \( \mathcal{L} \) the bound of Theorem 1 can only be attained by maximally entangled states, this can be translated into a Bell inequality whose Tsirelson bound is reached by such a state as we have particularly shown for a two-qutrit maximally entangled state. This could be applied for robust self-testing using the techniques developed in [31]. Several ideas will be further investigated in the future. Given a Bell inequality, it would be interesting to find a procedure to find the best form of \( G \) in (1) to obtain its quantum upper bound and when it can be optimal. Also, to characterize in general which behaviours in \( Q \setminus \mathcal{L} \) attain the bound in Theorem 1 and whether they only arise from maximally entangled states and use this further for robust self-testing. Last, it would be desirable to extend this approach to the multipartite setting.

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[34] Still, determining \( G_L \) and \( G_{\pm S} \) can be computationally hard as the number of vertices increases exponentially with the number of inputs.
APPENDIX A: PROOF OF THEOREMS 1 AND 2 AND INEQUALITIES (3) AND (4)

The proof of these results goes along similar lines so we will only provide full details in the first case. We restate again all of them for the sake of clarity.

**Theorem 1.** In every \((m_A m_B d_A d_B)\) scenario, if \(P \in Q\) then \(\|P\|_1 \leq \sqrt{m_A m_B}\).

**Proof.** As explained in the main text we have to prove that for every \(P \in Q\) it must hold that

\[
\langle P, G \rangle = \text{tr}(PG^T) = \sum_{abxy} P(ab|xy)G(ab|xy) \leq \|G\|_\infty \sqrt{m_A m_B} \quad \forall G \in \mathbb{R}^{n_A \times n_B},
\]

and that we will do it by showing that the inequality holds \(\forall P \in Q^1\). Such behaviours must fulfill \([1]\) that a \((n_A + n_B) \times (n_A + n_B)\) real positive semidefinite matrix \(\Gamma = \begin{pmatrix} Q & P \\ P^T & R \end{pmatrix}\) exists with \(Q_{ii} = P_A(i)\) and \(R_{jj} = P_B(j)\), where \(P_A(P_B)\) is a vector of \(\mathbb{R}^{m_A d_A}(\mathbb{R}^{m_B d_B})\) with entries given by \(P(a|x)\) \((P(b|y))\) with \(xa\) \((by)\) in lexicographical order \([10]\). Thus, defining \(W = \begin{pmatrix} 0 & G^T \\ G & 0 \end{pmatrix}\), for any given \(G\) the maximum value of \(\langle P, G \rangle\) attainable in \(Q\) cannot be larger than

\[
\max_{\Gamma} \text{tr}(\Gamma W)/2, \text{ subject to } \\
\Gamma \geq 0, \\
\text{tr}(D^A \Gamma) = P_A(i) \quad (i = 1, \ldots, n_A), \\
\text{tr}(D^B \Gamma) = P_B(j) \quad (j = 1, \ldots, n_B),
\]

where \(D^A = E_i \oplus 0_{n_B} (D^B = 0_{n_A} \oplus E_j)\) and \(E_i (E_j)\) a \(n_A \times n_A (n_B \times n_B)\) matrix whose only nonzero entry is the \(ii\) \((jj)\) with value 1. This is the primal form of a semi-definite program (SDP) \([2]\) with cost function \(p(\Gamma)\) and we will denote its solution by \(p(\Gamma^*)\). The dual form of this SDP corresponds to

\[
\min_x x^T \begin{pmatrix} P_A & P_B \end{pmatrix}, \text{ subject to } \text{diag}(x) - W/2 \geq 0,
\]

where \(x\) is a \(n_A + n_B\) real vector yielding the value \(d(x)\). By duality, for any feasible \(x\) (i.e. satisfying the constraint above), it must hold that \(p(\Gamma^*) \leq d(x)\). Thus, to finish the proof it suffices to construct a feasible \(x\) yielding the value \(d(x) = \|G\|_\infty \sqrt{m_A m_B}\). This is the case for \(x = \|G\|_\infty /2(\sqrt{m_B/m_A} 1_{n_A} + \sqrt{m_A/m_B} 1_{n_B})\) where \(\Gamma_n\) is the \(n\)-dimensional vector with all entries equal to one. To see that it is feasible amounts to checking that

\[
\left( \begin{array}{cc} \sqrt{m_B/m_A} & -G \\ -G^T & \sqrt{m_A/m_B} \end{array} \right) \geq 0.
\]

This is indeed true because, since the upper left corner in strictly positive definite, by Schur’s complement condition \([3]\) this is equivalent to

\[
\sqrt{m_A/m_B} \left( \|G\|_\infty 1_{n_B} - G^T G \right) \geq 0,
\]

which is obviously true given that the maximal eigenvalue of \(G^T G\) is precisely \(\|G\|_2^2\). \(\square\)

**Theorem 2.** In every \((m_A m_B d_A d_B)\) scenario, if \(P \in Q\) then

\[
\|M\|_1 \leq \sqrt{m_A m_B} \left( 1 - \sum_{ax} P(a|x)^2 - \sum_{by} P(b|y)^2 \right).
\]

**Proof.** As before, we are going to prove that \(\forall P \in Q\) and for any choice of \(G \in \mathbb{R}^{n_A \times n_B}\),

\[
\langle M, G \rangle \leq \|G\|_\infty \sqrt{m_A m_B} - \|G\|_\infty \sqrt{m_B / 2 m_A} \sum_{ax} P(a|x)^2 - \|G\|_\infty \sqrt{m_A / 2 m_B} \sum_{by} P(b|y)^2.
\]

The set \(Q^1\) is actually equivalent to the positive semidefiniteness of \(\Gamma = \begin{pmatrix} P_A & P_B^- \\ P_B^- & P^T_B \end{pmatrix}\) \([4]\), that is,

\[
\tilde{\Gamma} = \begin{pmatrix} \tilde{Q} & M \\ M^T & \tilde{R} \end{pmatrix} \geq 0,
\]

where now \(\tilde{Q}_{ii} = P_A(i) - P_A(i)^2\) and \(\tilde{R}_{jj} = P_B(j) - P_B(j)^2\). This leads to the primal SDP

\[
\max_{\tilde{\Gamma}} \text{tr}(\tilde{\Gamma} W)/2, \text{ subject to } \\
\tilde{\Gamma} \geq 0, \\
\text{tr}(D^A \tilde{\Gamma}) = P_A(i) - P_A(i)^2 \quad (i = 1, \ldots, n_A), \\
\text{tr}(D^B \tilde{\Gamma}) = P_B(j) - P_B(j)^2 \quad (j = 1, \ldots, n_B),
\]

with dual

\[
\min_x x^T \begin{pmatrix} P_A - P_A^2 & P_B - P_B^2 \end{pmatrix}, \text{ subject to } \text{diag}(x) - W/2 \geq 0,
\]

where the vectors \(P_{A,B}^2\) have entries \(P_A(i)^2\) and \(P_B(j)^2\). The same choice of \(x\) as in the previous proof does the job. \(\square\)

The result of \([5]\),

\[
\sum_{xy} G_{xy} A_x B_y \leq \|G\|_\infty \sqrt{m_A m_B} \quad \forall P \in Q,
\]

can be proved in the same way by noticing that behaviours in \(Q^1\) must fulfill \([1]\) that a \((m_A + m_B) \times (m_A + \)
Therefore for \( \hat{Q}_{xx} = 1 \) and \( \hat{R}_{yy} = 1 \). The modification
\[
\sum_{xy} G_{xy}(A_x B_y) - \langle A_x \rangle \langle B_y \rangle \leq \left| G \right|_\infty \sqrt{m_A m_B}
\]
follows from the fact that \( Q^1 \) is equivalent [1] to the positive semi-definiteness of
\[
\begin{pmatrix}
\frac{1}{\langle A \rangle} \langle B \rangle \\
\langle A \rangle^T \hat{Q} & C \\
(B)^T & C^T \hat{R}
\end{pmatrix}
\]
where \( \langle A \rangle \langle B \rangle \) is an \( m_A (m_B) \)-dimensional vector with entries \( \langle A_x \rangle \langle B_y \rangle \). By Schur’s complement condition this leads to
\[
\begin{pmatrix}
\hat{Q} & C \\
C^T & \hat{R}
\end{pmatrix} - \begin{pmatrix}
\langle A \rangle \\
\langle A \rangle^T \hat{Q} & C \\
(C)^T & \hat{R}
\end{pmatrix} \geq 0
\]
with \( \hat{Q}_{xx} = 1 - \langle A_x \rangle^2 \) and \( \hat{R}_{yy} = 1 - \langle B_y \rangle^2 \).

Finally, let us show that the condition of Theorem 1 is stronger than inequality (3), i.e.

Proposition 6. For every \( P \in NS \), if \( \|C\|_1 > \sqrt{m_A m_B} \), then \( \|P\|_1 > \sqrt{m_A m_B} \).

Proof. By permutation matrices, that leave the trace norm invariant, we can map \( P = \sum_{abxy} P(ab|xy|xa\langle yb| \) to \( P' = \sum_{abxy} P(ab|xy|ax\langle yb| \), which has now blocks given by
\[
P'_{ab} = \begin{pmatrix}
P(ab|11) & \cdots & P(ab|1m_B) \\
\vdots & \ddots & \vdots \\
P(ab|m_A) & \cdots & P(ab|m_B m_B)
\end{pmatrix} \in \mathbb{R}^{m_A \times m_B}.
\]
Therefore for \( d_A = d_B = 2 \), using Corollary 3 in [6], we obtain that
\[
\|P\|_1 = \left\| \left[ \begin{array}{c} P'_{11} \\ P'_{12} \\ P'_{21} \\ P'_{22} \end{array} \right] \right\|_1
\geq \frac{1}{2} \left\| \left[ \begin{array}{c} 1 \\ \vdots \\ 1 \\ \vdots \\ 1 \end{array} \right] \right\|_1 + \|C\|_1
\]
\[
= \frac{1}{2} \left\| \left[ \begin{array}{c} 1 \\ \vdots \\ 1 \end{array} \right] \right\|_1 + \|C\|_1
\]
\[
= \sqrt{m_A m_B} + \|C\|_1
\]
\[
= \sqrt{m_A m_B} + \|C\|_1
\]
\[
\frac{1}{2} \left\| \left[ \begin{array}{c} 1 \\ \vdots \\ 1 \end{array} \right] \right\|_1 + \|C\|_1
\]
\[
= \frac{\sqrt{m_A m_B} + \|C\|_1}{2}
\]

APPENDIX B: PROOF OF PROPOSITION 3 AND ESTIMATES FOR \( \|P_{PR}\|_1 \)

Proposition 3. In every \( (m_A m_B d_A d_B) \) scenario, if \( P \in \mathcal{L} \) then \( \|P\|_1 \leq \sqrt{m_A m_B} \), with equality for LDBs.

Proof. Every LDB is of the form \( D_i(ab|xy) = d_i^A(a|x)d_i^B(b|y) \) where the lists \( d_i^A(a|x) \) \( d_i^B(b|y) \) have \( m_A \) \( m_B \) entries equal to 1 and 0 otherwise. Hence,
\[
\|D_i\|_1 = \left\| \left( \sum_{ab} d_i^A(a|x) \right) \left( \sum_{by} d_i^B(b|y) \right) \right\|_1
\]
\[
= \left\| \sum_{ab} d_i^A(a|x) \right\|_2 \left\| \sum_{by} d_i^B(b|y) \right\|_2
\]
\[
= \sqrt{m_A m_B}.
\]
Notice that the fact that \( \|P\|_1 \leq \sqrt{m_A m_B} \) holds \( \forall P \in \mathcal{L} \) follows then by the convexity of the trace norm without the need of invoking Theorem 1.

To see that \( \|P_{PR}(2, d)\|_1 \geq \sqrt{5} \) (which leads to Theorem 4), we use again the mapping from \( P \) to \( P' \) as in the proof of Proposition 6. We therefore have
\[
\|P_{PR}(2, d)\|_1 = \|P'_{PR}(2, d)\|_1
\]
\[
= \frac{1}{d} \left\| \begin{pmatrix}
Z & 0 & \cdots & Y \\
Y & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & Y \\
0 & \cdots & 0 & Y \\
0 & \cdots & 0 & Y
\end{pmatrix} \right\|_1
\]
where
\[
Z = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}
\]
Hence, using the pinching inequality we obtain that
\[\|P_{PR}(2, d)\|_1 \geq \left( |d| |Z|_1 \right) / d = \sqrt{5}.\] To see that \( \|P_{PR}(2, d)\|_2 \leq 2\sqrt{2} \), notice that for the Frobenius norm \( \|P_{PR}(2, d)\|_2 = \sqrt{\text{tr}(P_{PR}(2, d) P_{PR}(2, d)^T)} = 2 \sqrt{d} \) and that \( \|X\|_1 \leq \sqrt{m} \|X\|_2 \) for any n x n matrix X. Similarly, for the fully nondeterministic boxes \( P_{PR}(m, 2) \) there are \( 2m^2 \) non-vanishing entries with value 1/2 [7]. Hence, \( \|P_{PR}(m, 2)\|_2 = m / \sqrt{2} \) and we obtain \( \|P_{PR}(m, 2)\|_1 \leq \sqrt{m} \) as claimed in the main text.

APPENDIX C: A BELL EXPRESSION WITH QUANTUM BOUND ATTAINED BY A MAXIMALLY ENTANGLED TWO-QUTRIT STATE

If a real square matrix \( P \) has singular value decomposition given by
\[
P = \sum_i \sigma_i u_i v_i^T = U \Sigma V^T,
\]
then \(|P|_1 = \text{tr}\Sigma = \text{tr}(PO)\) with \(O = U^T V\) orthogonal (as so are \(U\) and \(V\)). Thus, if we have a quantum behaviour such that \(|P|_1 = \sqrt{m_4 m_6}\), the matrix \(O\) obtained through the aforementioned prescription immediately yields a Bell expression which is maximized in \(Q\) by \(P\). This is because for every matrix \(|P|_1 = \max_O \text{tr}(PO)\) and otherwise we would have a contradiction with Theorem 1. This is the case for the behaviour arising from a maximally entangled two-qutrit state given in \([8, 9]\) for the setting (2233) (i.e. \(|P|_1 = 2\)).

With this, one finds that a Bell expression which is maximized by this behaviour over \(Q\) is given by \(G(\Phi_3^+) = O^T\) with \([11]\)

\[
O = \begin{pmatrix}
\frac{2+\sqrt{3}}{6} & \frac{2-\sqrt{3}}{6} & \frac{1}{6} & \frac{2+\sqrt{3}}{6} & \frac{-1}{6} & \frac{2-\sqrt{3}}{6} \\
\frac{-1}{6} & \frac{2+\sqrt{3}}{6} & \frac{2-\sqrt{3}}{6} & \frac{2+\sqrt{3}}{6} & \frac{-1}{6} & \frac{2-\sqrt{3}}{6} \\
\frac{2-\sqrt{3}}{6} & \frac{-1}{6} & \frac{2+\sqrt{3}}{6} & \frac{-1}{6} & \frac{2-\sqrt{3}}{6} & \frac{2+\sqrt{3}}{6} \\
\frac{2+\sqrt{3}}{6} & \frac{-1}{6} & \frac{2-\sqrt{3}}{6} & \frac{2+\sqrt{3}}{6} & \frac{-1}{6} & \frac{2-\sqrt{3}}{6} \\
\frac{-1}{6} & \frac{2-\sqrt{3}}{6} & \frac{2+\sqrt{3}}{6} & \frac{-1}{6} & \frac{2-\sqrt{3}}{6} & \frac{2+\sqrt{3}}{6} \\
\frac{-1}{6} & \frac{2-\sqrt{3}}{6} & \frac{2+\sqrt{3}}{6} & \frac{-1}{6} & \frac{2-\sqrt{3}}{6} & \frac{2+\sqrt{3}}{6}
\end{pmatrix}
\]

(13)

Notice that this Bell inequality separates \(L\) from \(Q\) as it is straightforward to find that the maximal value of \(G(\Phi_3^+)\) under \(L\) is \((3\sqrt{3} + 5)/6 \simeq 1.70\).

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[10] Other entries of \(Q\) and \(R\) have to be fixed to zero. See [1] for details.
[11] In order to have a symmetrical Bell expression we have used the reduced singular value decomposition of \(P\). Hence, \(U\) and \(V\) are not orthogonal (they are not square) and nor is \(O\). Still, it holds that \(G(\Phi_3^+)_Q = 2\) due to inequality (1) in the main text as \(||G(\Phi_3^+)||_\infty = ||O||_\infty = 1\).

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