Extremal Tsirelson Inequalities

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It is well known that the set of statistics that can be observed in a Bell-type experiment is limited by quantum theory. Unfortunately, tools are missing to identify the precise boundary of this set. Here, we propose to study the set of quantum statistics from a dual perspective. By considering all Bell expressions saturated by a given realization, we show that the Clauser-Horne-Shimony-Holt expression can be decomposed in terms of extremal Tsirelson inequalities that we identify. This brings novel insight into the geometry of the quantum set in the (2,2,2) scenario. Furthermore, this allows us to identify all the Bell expressions that are able to self-test the Tsirelson realization.

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Introduction.-Quantum physics predicts the existence of statistics in a Bell-type experiment which are nonlocal in the sense that they can violate a Bell inequality [1]. The observation of this striking physical property has raised awareness on the importance of the statistical distributions that can be observed in a Bell scenario upon measurement of a quantum system, which form the set of quantum behaviors—or simply the quantum set Q. By defining statistics that are experimentally realizable, this set plays a central role in quantum information science, with applications ranging from foundational questions to device-independent information protocols [2-7]. Indeed, every quantum realization, consisting of a density matrix and local measurements on some Hilbert spaces of arbitrary dimension, generates statistics according to Born's rule which belong to the quantum set. Given a statistical distribution, it is however generally a difficult question to determine which quantum realization may generate it, or even whether the distribution belongs to the quantum set in the first place.

The Navascués-Pironio-Acín hierarchy of semidefinite programming offers a tool to tackle this question in terms of a family of statistical sets converging to the quantum set from the outside [8,9]. However, this construction involves additional variables whose value is *a priori* unknown, and the level of the hierarchy which must be reached in order to provide a definitive answer is unknown even in the simplest Bell scenario. Another approach is motivated by the convexity of the quantum set and involves decomposing quantum behaviors in terms of extremal points. Despite much effort, a complete description of extremal quantum behaviors remains to be discovered [10–12]. Here, we take a different path, also enabled by Q's convexity property, which consists in studying its dual set Q^* .

The dual of the quantum set encodes the Tsirelson bounds of all possible Bell inequalities [13,14]. Describing it is therefore as challenging as finding the quantum bound of an arbitrary Bell inequality, but is also as important, since quantum bounds play a key role in many quantum information results [15–17]. The duality perspective already brings insight into the local and no-signaling sets, which are the two other major sets of interest in Belltype experiments. Namely, for Bell scenarios with binary inputs and outputs it was shown that the local set, describing statistical distributions compatible with a local hidden variable model, is dual to the no-signaling set, whose behaviors are only limited by the condition that the parties cannot learn each other's inputs [18]. In other words, every extremal (or 'tight') Bell inequality in this scenario is in one-to-one correspondence with an extremal point of the no-signaling polytope.

Unlike its local and no-signaling counterparts, the quantum set is not a polytope and little is known about its dual picture. In the simplest Bell scenario exhibiting the nonlocal property of quantum physics, with 2 parties, 2 inputs, and 2 outputs, the quantum set belongs to a space of dimension 8. A first result concerns the subset Q_c with uniformly random marginal statistics, corresponding to a subspace of dimension 4. It was recently shown that this subset is self-dual, i.e., $Q_c \cong Q_c^*$ [18,19]. This striking property sets the quantum set apart from both the local and the no-signaling sets. In fact, the analytical descriptions of Q_c and Q_c^* are fully known within this subspace: a first explicit description of the quantum set in the subspace of vanishing marginals was provided in [10,13,20]; see also [19,21,22] for explicit descriptions of its (isomorphic) dual.

Here, we study the dual of the quantum set in the full eight-dimensional space. Specifically, we determine analytically all elements of the dual which are related to the Tsirelson point, the unique quantum point maximally violating the Clauser-Horne-Shimony-Holt (CHSH) inequality [23]. This allows us to describe for the first time a complete face of the dual quantum set Q^* 's boundary. In turn, this provides a tight first order

description of the quantum set around this maximally nonlocal point.

Dual of the quantum set.—In a bipartite Bell experiment, two parties obtain outcomes a and b upon performing measurements x and y respectively. A behavior P(ab|xy) in this scenario belongs to the quantum set Q iff there exists Hilbert spaces \mathcal{H}_A , \mathcal{H}_B , a density matrix $\rho \ge 0$ with $tr\rho = 1$ acting on their tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$, and POVMs $M_{a|x}, N_{b|y} \ge 0$ with $\sum_a M_{a|x} = 1$, $\sum_b N_{b|y} = 1$ such that $P(ab|xy) = tr(M_{a|x} \otimes N_{b|y}\rho)$. Since the dimensions of the Hilbert spaces \mathcal{H}_A and \mathcal{H}_B are not bounded, any convex mixture $\lambda P_1 + (1 - \lambda)P_2$ with $\lambda \in [0, 1]$ of two behaviors P_1 and P_2 in Q can be obtained by combining the two corresponding realizations into larger Hilbert spaces, and therefore Q is convex [24].

By taking into account the normalization and no-signaling conditions, the 16 conditional probabilities P(ab|xy)can be expressed simply in terms of eight linearly independent ones [25,26], which can be represented by the corresponding table of correlators

$$\boldsymbol{P} = \frac{1}{\frac{\langle A_0 \rangle}{\langle A_1 \rangle}} \frac{\langle B_0 \rangle}{\langle A_0 B_0 \rangle} \frac{\langle B_1 \rangle}{\langle A_0 B_1 \rangle}. \tag{1}$$

Here, $A_x = M_{0|x} - M_{1|x}$ and $B_y = N_{0|y} - N_{1|y}$ are observables with ± 1 eigenvalues. This allows one to define the dual of the quantum set Q^* in \mathbb{R}^8 as the set of all Bell expressions β whose quantum maximum is smaller than a constant, e.g., 1 (see [27], Sec. A]:

$$\mathcal{Q}^* = \{ \boldsymbol{\beta} \in \mathbb{R}^8 \colon \boldsymbol{\beta} \cdot \boldsymbol{P} \le 1, \ \forall \ \boldsymbol{P} \in \mathcal{Q} \}.$$
(2)

Since the double dual of a cone is the closure of the initial cone, the description of Q^* is equivalent to the description of Q itself, and any insight on Q^* is an insight on Q as well.

Note that all elements of Q^* with

$$\boldsymbol{\beta} \cdot \boldsymbol{P} = 1 \tag{3}$$

for some $P \in Q$ are Bell expressions defining supporting hyperplanes of the quantum set Q. Such inequalities provide a description of the quantum set around the point P to first order. More generally, the dual of the quantum set Q^* being convex, admits extremal points, which are of particular interest. An example of an extremal point of Q^* is the positivity constraint $P(ab|xy) \ge 0$. However, this point is not specific to the quantum dual as it is shared with every other physically meaningful dual, including the local and no-signaling duals. In the remainder of this manuscript, we are going to identify nontrivial extremal points of Q^* .

The Tsirelson behavior.—The Tsirelson point is given by the following table of correlators

$$\boldsymbol{P}_{T} = \frac{\frac{1}{0} \quad \frac{0}{\sqrt{2}} \quad \frac{1}{\sqrt{2}}}{0 \quad \frac{1}{\sqrt{2}} \quad -\frac{1}{\sqrt{2}}}.$$
(4)

This point is particularly remarkable because it is the only point in Q that achieves the maximal quantum value of the CHSH Bell inequality $\langle \beta_{\text{CHSH}} \rangle \leq 2$ [29]. Furthermore, this point is extremal in Q, and it can only be realized by performing complementary measurements on a maximally entangled state, i.e., the point P_T self-tests the quantum realization [17]:

$$|\phi^{+}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle),$$

 $A_{x} = \frac{Z_{A} + (-1)^{x}X_{A}}{\sqrt{2}}, \qquad B_{0} = Z_{B}, \qquad B_{1} = X_{B}.$ (5)

As shown in Eq. (4), the Tsirelson point has vanishing marginals, and when considering Q_c , the quantum set within the subspace of vanishing marginals, i.e., with $\langle A_x \rangle = \langle B_y \rangle = 0$, it is known that this point is only exposed by the CHSH inequality. In other words, the hyperplane $\langle \beta_{\text{CHSH}} \rangle = 2\sqrt{2}$ is the only linear function of $\{\langle A_x B_y \rangle\}_{x,y}$ such that $H \cap Q_c = \{P_T\}$. Recent numerical results suggest however that this may not be the case outside the subspace of vanishing marginals [30]. In the following, we identify all Bell expressions that are maximized by the Tsirelson point.

Bell expressions for the Tsirelson point.—In general, all possible Bell expressions can be parametrized by eight real coefficients a_x, b_y, c_{xy} for $x, y \in \{0, 1\}$ and be written in terms of formal polynomials [21] as

$$\beta = a_0 A_0 + a_1 A_1 + b_0 B_0 + b_1 B_1 + c_{00} A_0 B_0 + c_{10} A_1 B_0 + c_{01} A_0 B_1 + c_{11} A_1 B_1.$$
(6)

In order to find restrictive conditions that ensure that β has quantum bound 1 and verifies Eq. (3) for the Tsirelson point P_T , we make use of the variational method [21,31,32] and consider the Bell operator corresponding to these polynomials for the choice of measurements of Eq. (5). In general, this operator is given by

$$\hat{S} = p_1 Z_A + p_2 X_A + p_3 Z_B + p_4 X_B + p_5 Z_A Z_B + p_6 X_A X_B + p_7 Z_A X_B + p_8 X_A Z_B, \quad (7)$$

where parameters p_r are linear combinations of parameters a_x, b_y, c_{xy} .

For any given state, the value of the Bell inequality is then given by $\langle \psi | \hat{S} | \psi \rangle$. Since \hat{S} is a real hermitian operator, its eigenvalues are real and $\beta \in Q^*$ imposes that all of its eigenvalues are smaller than 1. The condition Eq. (3) for P_T then implies that $|\phi^+\rangle$ is an eigenstate of \hat{S} of eigenvalue 1, i.e., $\hat{S}|\phi^+\rangle = |\phi^+\rangle$, which grants the following conditions on the parameters p_r :

$$p_1 + p_3 = 0,$$
 $p_5 + p_6 = 1,$
 $p_2 + p_4 = 0,$ $p_7 - p_8 = 0.$ (8)

Taking these equations into account, we can now rewrite a new parametrization:

$$\beta = r_0 \left(\frac{A_0 + A_1}{\sqrt{2}} - B_0 \right) + r_1 \left(\frac{A_0 - A_1}{\sqrt{2}} - B_1 \right) + r_2 \left(\frac{A_0 + A_1}{\sqrt{2}} B_1 + \frac{A_0 - A_1}{\sqrt{2}} B_0 \right) + \lambda \frac{A_0 + A_1}{\sqrt{2}} B_0 + (1 - \lambda) \frac{A_0 - A_1}{\sqrt{2}} B_1,$$
(9)

where $r_0, r_1, r_2, \lambda \in \mathbb{R}$ are the remaining free parameters.

Perturbative restriction.—Now, remember that we require that no other quantum point gives a value larger than 1 for this Bell expression. In particular, the function $\beta \cdot P_{\theta,a_x,b_y}$ should admit a local maxima at P_T , where

$$\boldsymbol{P}_{\theta,a_x,b_y} = \frac{\frac{1}{c_{2\theta}c_{a_1}}}{\frac{c_{2\theta}c_{a_2}}{c_{2\theta}c_{a_2}}} \frac{c_{2\theta}c_{b_1}}{c_{a_x}c_{b_y} + s_{2\theta}s_{a_x}s_{b_y}}, \quad \theta, a_x, b_y \in \mathbb{R}$$
(10)

are the statistics resulting from measuring the two-qubit state $|\phi_{\theta}\rangle = c_{\theta}|00\rangle + s_{\theta}|11\rangle$ in the Z - X plane, and $c_{\varphi} \coloneqq \cos(\varphi)$, $s_{\varphi} \coloneqq \sin(\varphi)$ denote the cosine and sine functions. This condition gives a set of five linear equations:

$$0 = \beta \cdot \frac{\partial \boldsymbol{P}_{\theta, a_x, b_y}}{\partial \theta} = \beta \cdot \frac{\partial \boldsymbol{P}_{\theta, a_x, b_y}}{\partial a_x} = \beta \cdot \frac{\partial \boldsymbol{P}_{\theta, a_x, b_y}}{\partial b_y} \quad (11)$$

which reduce to

$$\lambda = 1/2, \qquad r_2 = 0.$$
 (12)

The search space for the Bell inequalities is thus reduced to

$$\beta_{r_0,r_1} = r_0 \left(\frac{A_0 + A_1}{\sqrt{2}} - B_0 \right) + r_1 \left(\frac{A_0 - A_1}{\sqrt{2}} - B_1 \right) + \frac{1}{2\sqrt{2}} \beta_{\text{CHSH}}, \qquad r_0, r_1 \in \mathbb{R},$$
(13)

where $\beta_{\text{CHSH}} = (A_0 + A_1)B_0 + (A_0 - A_1)B_1$. As shown in [27], Sec. C, further order perturbations can be considered to reduce the range of the parameters r_0 , r_1 , but it turns out to be more restrictive at this stage to eliminate parameters based on the local bound of the Bell expressions. Indeed,

any β_{r_0,r_1} with a local bound larger than 1 also admits a quantum value larger than 1 (and hence larger than the value provided by measuring the $|\phi^+\rangle$ state).

Local bounds.—Since the convex combination of two Bell expressions with a local bound smaller than 1 also has a local bound smaller than 1, the set of Bell expressions β_{r_0,r_1} with a local bound smaller than 1 forms a convex region of the r_0 , r_1 plane. Furthermore, the local maxima of a Bell expression is reached at one of the 16 extremal points of the local polytope. These points are given by

$$L_{ijkl} = \frac{\frac{1}{k}}{\frac{ik}{l}} \frac{j}{jk}, \qquad i, j, k, l \in \{-1, 1\}.$$
(14)

The convex region of expressions of the form Eq. (13) with a local maxima smaller than 1 is thus given by all points (r_0, r_1) satisfying the conditions $\beta_{r_0, r_1} \cdot L_{ijkl} \leq 1$. The intersection of these half planes defines a polytope, namely, a regular octagon, whose eight summit are given by (see Fig. 1)

$$\left\{ \left(1 - \frac{1}{\sqrt{2}}\right) R^{k}_{\frac{\kappa}{4}}(1,0), k \in [\![0,7]\!] \right\},$$
(15)

where $R_{(\pi/4)}$ is the rotation of angle $\pi/4$ in the (r_0, r_1) plane. Any Bell expression outside this octagon has a local bound larger than 1, and thus is not maximized by P_T .

Quantum bounds.—Having excluded a range of Bell expressions β_{r_0,r_1} from their local bound, we need to compute the Tsirelson bound of the expressions inside the octagon. To formalize this problem, let us consider the



FIG. 1. Face of Q^* in the two-dimensional affine slice defined by β_{r_0,r_1} for real parameters r_0, r_1 . The red point in the middle, the normalized CHSH expression, is non-extremal: it can be decomposed in terms of the eight summits of the octagon, which are extremal Tsirelson inequalities.

algebra of quantum operators \mathcal{R} made of arbitrary products of A_x and B_y . The only generating rules of this algebra are that, for all x, y, $A_x^2 = B_y^2 = 1$ and $[A_x, B_y] = 0$. We know that a sufficient condition to have $\beta \leq 1$ is that $1 - \beta$ is a sum of squares (SOS) in \mathcal{R} :

$$1 - \beta = \sum_{s} O_{s}^{\dagger} O_{s}, \qquad O_{s} \in \mathcal{R}.$$
 (16)

This is known as an SOS relaxation [33,34]. However, the search space \mathcal{R} is of infinite dimension. Since an SOS decomposition of the form of Eq. (16) where O_s are restricted to a set subspace $\mathcal{T} \subset \mathcal{R}$ still provides a valid bound, a common approach to tackle this problem consists in considering operators O_s within a chosen relaxation level \mathcal{T} , such as the set of all polynomials of A_x and B_y of a given degree. But even this quickly results in a large problem.

To further reduce the SOS search space, let us identify a relevant subspace of \mathcal{T} in which the operators O_s should be chosen. Let us consider the case where a SOS decomposition exists. For the implementation of the Tsirelson realization, this would imply

$$0 = \sum_{s} \langle \phi^{+} | \overline{O_{s}}^{\dagger} \overline{O_{s}} | \phi^{+} \rangle = \sum_{s} || \overline{O_{s}} | \phi^{+} \rangle ||^{2}, \quad (17)$$

where $\overline{O_s}$ is the specific implementation of the operator O_s using measurements of Eq. (5). Since all terms on the righthand side of the above equation are positive, this implies that for all s, $\overline{O_s} |\phi^+\rangle = 0$, i.e., that all $\overline{O_s}$ are nullifying operators of $|\phi^+\rangle$ [21,35]. This condition restricts the operators O_s to

$$\mathcal{A}_{\mathcal{T}} = \{ O \in \mathcal{T} : \bar{O} | \phi^+ \rangle = 0 \}.$$
(18)

For a finite relaxation \mathcal{T} , let us consider a generating sequence $\{N_s\}_s$ of $\mathcal{A}_{\mathcal{T}}$ and denote by \vec{N} the vector of elements N_s . All elements in $\mathcal{A}_{\mathcal{T}}$ can thus be written as $\vec{w} \cdot \vec{N}$ where \vec{w} is a real vector. A valid SOS decomposition in \mathcal{T} can then be written as

$$1 - \beta = \sum_{s} O_s^{\dagger} O_s = \vec{N}^{\dagger} \sum_{s} \vec{w}_s^{\dagger} \vec{w}_s \vec{N} = \vec{N}^{\dagger} \cdot W \cdot \vec{N}, \quad (19)$$

where $W = \sum_{s} \vec{w}_{s}^{\dagger} \vec{w}_{s}$ is a positive matrix. We see that the problem of obtaining an SOS decomposition, Eq. (16), reduces to finding whether there exists a positive matrix $W \succeq 0$ such that

$$1 - \beta = \vec{N}^{\dagger} \cdot W \cdot \vec{N}. \tag{20}$$

If such a matrix W can be found, we say it is a certificate of the inequality β .

Different relaxations \mathcal{T} could be considered here. The first order relaxation $\mathcal{T}_{1+A+B} = \{1, A_0, A_1, B_0, B_1\}$ only

gives a certificate for the CHSH inequality. The relaxation at the almost quantum level [36], $\mathcal{T}_{1+A+B+AB} = \mathcal{T}_1 \cup \{A_x B_y, x, y \in \{0, 1\}\}$ can also be computed numerically and gives a certificate for a disk in the (r_0, r_1) plane of center (0,0) and radius $(1/4\sqrt{2})$, cf. [27], Sec. C. The next relaxation is given by

$$\mathcal{T}_{1+A+B+AB+ABB'} = \mathcal{T}_{1+AB} \cup \{A_x B_y B_{y'}, y \neq y'\}.$$
 (21)

We can show analytically that a certificate can be found for the inequality $\beta_{1-1/\sqrt{2},0}$ at this level of relaxation [27], Sec. B. This ensures that the Bell expression

$$\beta_T = \left(1 - \frac{1}{\sqrt{2}}\right) \left(\frac{A_0 + A_1}{\sqrt{2}} - B_0\right) + \frac{\beta_{\text{CHSH}}}{2\sqrt{2}} \quad (22)$$

is maximized by the Tsirelson point. Since we already concluded that a larger value of r_0 admits a local value larger than 1, this bound for $r_1 = 0$ is the best we could have hoped for. One can check that this inequality is an extremal point of Q^* , that it is exposed, in the sense that the quantum set admits a point which only saturates this Tsirelson inequality [27], Sec. A, and that it is only maximized by 3 extremal points of Q: P_T and two deterministic realizations [27], Sec. D.

To analyze the rest of the octagon, we make use of some symmetries of the problem. Both the family of Bell expressions β_{r_0,r_1} and the set Q are preserved by several discrete symmetries. One of them is described by the following action:

$$S: (r_0, r_1) \to R_{\frac{\pi}{4}}(r_0, r_1), \qquad \begin{cases} A_0 \to -B_1, & A_1 \to -B_0, \\ B_0 \to -A_0, & B_1 \to A_1. \end{cases}$$
(23)

Because of this symmetry, the quantum bound of any Bell expression with parameters $(r_0, r_1) \in \mathbb{R}^2$ can be computed by looking at the bound of the inequality with parameters rotated by $\pi/4$. This ensures that the quantum bounds of the eight inequalities $S^k \cdot \beta_T$ of polar coordinates $[1 - (1/\sqrt{2}), k(\pi/4)]$ for $k \in [0, 7]]$ are also 1. Therefore, the octagon is exactly the convex region of quantum bound equal to 1. This completes the characterization of the slice β_{r_0,r_1} (see Fig. 1).

Interestingly, the CHSH inequality lies in the middle of this dual face. Therefore, the CHSH inequality is not an extremal Tsirelson inequality. In particular, we can write it as the convex mixture

$$\beta_{\text{CHSH}} = \frac{1}{2} \left(\beta_T + S^4 \cdot \beta_T \right). \tag{24}$$

Note that this description is not unique because β_{CHSH} lies on a face of Q^* of dimension 2.



FIG. 2. Three-dimensional projection of the local polytope (in red) and of the quantum set of correlations (red and blue). The only point reaching the *z* value of 1 is the Tsirelson realization. This point lies on top of an octagonal-based pyramid whose eight facets correspond to the inequalities $S^k \cdot \beta_T$.

From the point of view of the quantum set, this means that the Tsirelson point P_T is an exposed extremal point of Q with dimension pair (0,2), i.e., with a face dimension of 0 and a dual dimension of 2 [27], Sec. A. Furthermore, it is exposed by all the inequalities on the inside of the octagon (see Fig. 2). In fact, any Bell expression inside the octagon can be written as a convex combination of the CHSH expression and an expression β_b on the border of the octagon: $\beta = p\beta_{\text{CHSH}}/2\sqrt{2} + (1-p)\beta_b$, where $p \in (0, 1]$. If a point **P** verifies $\beta \cdot \mathbf{P} = 1$, then it implies $\beta_{\text{CHSH}} \cdot \mathbf{P} =$ $2\sqrt{2}$ and the self-testing result of β_{CHSH} implies that $P = P_T$. From the self-testing point of view, this means that any inequality inside the octagon self-tests the quantum realization of Eq. (5) associated to the Tsirelson point. As far as inequalities on the border of the octagon are concerned, those are also maximized by local points and as such cannot provide a self-test of the realization.

Conclusion.—In this Letter, we studied the quantum set Q from a dual perspective. In particular, we derived constructively all the Bell expressions that the Tsirelson point P_T maximizes. This provides fresh insight on the geometry of the quantum set. In particular, we show analytically that P_T is an extremal point of Q of dual dimension 2 that lies at the top of a pyramid. We identify eight new exposed extremal points of Q^* , all of dual dimension 2 as well, thus fully describing a face of Q^* of dimension 2. In turn, this allows us to describe all the Bell expressions that are able to self-test the Tsirelson realization. It would be interesting to find out whether it is a generic property of extremal quantum statistics to have a nonzero dual dimension.

Our work also sheds light on the relation between Q and Q^* . In [18], a map was introduced to prove that $\mathcal{L}^* \cong \mathcal{NS}$

and it was proven that this map also sends the subset Q_c with uniformly random marginals statistics to its dual. However, since this map sends the extremal point P_T onto β_{CHSH} , which admits the decomposition Eq. (24), it cannot be used to map Q to Q^* . While other maps could be found, analysis such as ours might help proving that the quantum set Q is not self-dual, making Q^* a set of physical interest with a possibly very different geometrical structure.

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