From Bell Inequalities to Tsirelson's Theorem: A Survey

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Abstract

The first part of this paper contains an introduction to Bell inequalities and Tsirelson's theorem for the non-specialist. The next part gives an explicit optimum construction for the "hard" part of Tsirelson's theorem. In the final part we describe how upper bounds on the maximal quantum violation of Bell inequalities can be obtained by an extension of Tsirelson's theorem, and survey very recent results on how exact bounds may be obtained by solving an infinite series of semidefinite programs.

Keywords: Quantum information, Quantum computation, Quantum correlation, Bell inequality, Non-local games

1 Introduction

Correlations between observed measurements are a fundamental resource in quantum information. In his seminal 1964 paper, Bell [4] demonstrated an inequality that must be satisfied by correlations obtained classically, but may be violated by a quantum correlation experiment. Subsequently, the term *Bell inequalities* has come to describe the set of inequalities that characterize correlations that can be obtained between events that can be well described by classical physics. Since the 1980s, a series of experimental results have been published that apparently demonstrate that quantum correlations do in fact violate Bell inequalities [12]. This raises the question of whether a "good" mathematical characterization of quantum correlation vectors can be obtained.

The first part of the paper is intended for the non-specialist. We begin by giving a survey of classical correlations, showing that they can be characterized using the well studied subject of L^1 -embeddings. Next we consider quantum correlations and give a statement of Tsirelson's theorem [5], which gives a partial characterization for the 2-party case. Interestingly, as we show, this characterization can be restated in terms of L^2 -embeddings. Tsirelson's theorem has found many applications in quantum information, but a direct constructive proof of his theorem is not readily available. Although this theorem is powerful,

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even in the two-party case it does not solve the characterization problem completely. We discuss this, and give an additional necessary condition based on no-signalling. In many applications of Tsirelson's theorem it is necessary to construct a quantum realization for a given correlation vector. An explicit construction is not given in his paper, but we give one here. We begin by giving a simple construction for the two dimensional case of Tsirelson's theorem, which uses a two qubit state. This includes introducing many of the ideas needed for the general construction.

In the second part of the paper, we give a new general construction, that is, states and operators which can represent all correlation functions. Our method is related to the theory of stabilizer states. We also demonstrate the optimality of this result, and give a scheme for a low dimensional approximation of an optimal representation.

In the third part of the paper we discuss the problem of finding the maximum violation of a Bell inequality. We see that semidefinite programming (SDP) plays a crucial role in this optimization problem, and relate it to the results given earlier in the paper. Finally we review some very recent work involving an infinite hierarchy of SDPs that gives a non-polynomial time method of characterizing Bell inequalities and finding maximum violations.

2 Classical correlations

Let $A_1, ..., A_n$ be a collection of n 0/1 valued random variables that belong to a common joint probability distribution. For $1 \le i < j \le n$, we define new random variables $A_i \triangle A_j$ that are one when $A_i = A_j$ and zero otherwise. Denote by $\langle A \rangle$ the expected value of a random variable A. The full correlation vector x based on $A_1, ..., A_n$ is the vector of length N = n + n(n-1)/2 given by the expected values:

$$x = (\langle A_i \rangle, \langle A_i \triangle A_j \rangle) \equiv (\langle A_i \rangle_{1 \le i \le n}, \langle A_i \triangle A_j \rangle_{1 \le i < j \le n}).$$

Note that each element of the above vector lies between zero and one. Now consider any vector $x = (x_1, ..., x_n, x_{12}, ..., x_{n-1,n}) \in [0,1]^N$ indexed as above, which we will call an *outcome*. We consider two related computational questions:

Recognition. When is an outcome x a full correlation vector?

Optimization. For any $c \in \mathbb{R}^N$ what is the maximum value of c^Tx over all possible full correlation vectors x?

It turns out that the recognition problem is NP-complete, and the optimization problem is NP-hard. This follows from the fact that the set of full correlation vectors is in fact the cut polytope CUT_{n+1} defined on the complete graph K_{n+1} . This polytope is defined as the convex hull of the 2^N full correlation vectors obtained by deterministically setting each random variable A_i to either zero or one. For details of the above and other facts about cut polytopes, see the book by Deza and Laurent [10]. For a vector $u = (u_1, ..., u_d)$ the L_1 -norm of u is given by $||u||_1 = \sum_{i=1}^d |u_i|$. We have the following well-known characterization of the cut polytope.

L_1 -characterization of full correlation vectors.

The following two statements are equivalent:

• An outcome $x \in [0,1]^N$ is a full correlation vector.

• There exist vectors $u^i \in \mathbb{R}^d$, $1 \leq i \leq n$, $d \leq N$, for which

$$x_i = ||u^i||_1, \quad x_{ij} = ||u^i - u^j||_1, \quad 1 \le i < j \le n.$$

Full correlation vectors provide an adequate model for correlations obtained in physical experiments at the classical level. Let us call the random variables observables. For example, with $n=3,\,A_1,\,A_2,\,A_3$ could obtain the value one if a given McGill student has blond hair, weighs more than 80 kg or is more than 180cm high, respectively. We could obtain a full correlation vector by determining these three observables for all McGill students.

In a quantum setting, things are very different. Firstly, it is difficult to apply the above model directly since at the quantum level it may be impossible to measure directly different observables for a given particle. Therefore the above model is replaced by a bipartite setting where the 0/1 random variables (observables) are labelled $A_1, ..., A_m$ and $B_1, ..., B_n$ respectively.

The (bipartite) correlation vector x based on random variables $A_1, ..., A_m$ and $B_1, ..., B_n$ is the vector of length M = m + n + mn given by the expected values:

$$x = (\langle A_i \rangle, \langle B_j \rangle, \langle A_i \triangle B_j \rangle)$$

$$\equiv (\langle A_i \rangle_{1 \le i \le m}, \langle B_j \rangle_{1 \le j \le n}, \langle A_i \triangle B_j \rangle_{1 \le i \le m, 1 \le j \le n}).$$
(1)

As we will be concerned only with the bipartite case, we will simply use the term correlation vector where no confusion arises. As before, we call any vector $x \in [0,1]^M$ indexed as in (1) an *outcome*. Again we may define a polytope by considering the convex hull of the 2^{m+n} correlation vectors formed by letting each of the m+n random variables take value either zero or one. This polytope is called the Bell polytope $B_{m,n}$ and was apparently first considered by Froissart [13]. It turns out the membership and optimization problems given above are still NP-complete and NP-hard respectively (for references, see, e.g., [2]). The characterization theorem generalizes in a natural way.

L_1 -characterization of bipartite correlation vectors.

The following two statements are equivalent:

- An outcome $x \in [0,1]^M$ is a bipartite correlation vector.
- There exist vectors $u^i, v^j \in \mathbb{R}^d$, $1 \le i \le m$, $1 \le j \le n$, $d \le M$, for which

$$x_i = ||u^i||_1, \quad x_{m+j} = ||v^j||_1, \quad x_{ij} = ||u^i - v^j||_1.$$

The Bell polytope has been much studied. Valid inequalities for the $B_{m,n}$ are often called Bell inequalities, although here we will reserve this term for the facets of $B_{m,n}$. These inequalities have been studied by many researchers, see for example [8], [22], [29]. The CHSH inequality is the only non-trivial facet of B(2,2) and is given by

$$\langle A_1 \triangle B_1 \rangle - \langle A_1 \triangle B_2 \rangle - \langle A_2 \triangle B_1 \rangle - \langle A_2 \triangle B_2 \rangle \le 0$$

or equivalently

$$x_{11} - x_{12} - x_{21} - x_{22} \le 0. (2)$$

Although few Bell inequalities were known until recently, much is known about facets of the cut polytope, including several large classes of facets. In [1] a method is given to generate Bell inequalities from facets of the cut polytope, producing a large number of new inequivalent Bell inequalities.

The correlation vector with m = 2, n = 2 given by

$$x = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{2 + \sqrt{2}}{4}, \frac{2 - \sqrt{2}}{4}, \frac{2 - \sqrt{2}}{4}, \frac{2 - \sqrt{2}}{4})$$
(3)

clearly violates the CHSH inequality (2), so it follows there is no joint distribution function for the four random variables. This correlation vector cannot arise as the result of an experiment for which the rules of classical physics apply. An outstanding prediction of quantum theory, apparently confirmed by numerous experiments, is that this correlation vector can arise from observations at the quantum level. This fact has lead to many surprising applications in quantum information theory, see for example Cleve et al.[7]. It raises the issue of whether there is a good characterization of such quantum correlation vectors, the topic of the rest of the paper.

3 Quantum correlations

The postulates of quantum theory give a complete statistical description of the outcome of experiments at the quantum level. A two party quantum correlation experiment can be described by a quantum state and set of observables $A_1, ..., A_m, B_1, ...B_n$ on a bipartite Hilbert space. It is assumed the two parties are spatially separated and that the observations are performed essentially simultaneously, so that there is insufficient time for the parties to communicate. For a given experimental outcome, the vector x defined by (1) is called a quantum correlation vector. The description given by the postulates does not appear to provide any tractable method to answer the recognition, optimization and characterization questions when applied to quantum correlation vectors. Such answers are provided, however, for one important case by a theorem of Tsirelson. A quantum correlation function is a vector $y \in \mathbb{R}^{mn}$ defined by taking the last mn coordinates of a quantum correlation vector, i.e.,

$$y = (\langle A_i \triangle B_j \rangle) \equiv (\langle A_i \triangle B_j \rangle_{1 \le i \le m, 1 \le j \le n}). \tag{4}$$

Tsirelson's Theorem (0/1 version)[5] [27].

The following three statements are equivalent:

- $y = (\langle A_i \triangle B_j \rangle) \in [0, 1]^{mn}$ is a quantum correlation function.
- $x = (1/2, 1/2, ..., 1/2, \langle A_i \triangle B_j \rangle) \in [0, 1]^M$ is a quantum correlation vector.
- There exist vectors $u^i, v^j \in \mathbb{R}^d$, $1 \leq i \leq m$, $1 \leq j \leq n$, $d \leq m+n$, for which

$$x_i = ||u^i|| = \frac{1}{2}, \quad x_{m+j} = ||v^j|| = \frac{1}{2}, \quad x_{ij} = ||u^i - v^j||.$$

where $||u|| \equiv u^T u$.

We call an experimental outcome unbiased if for all i and j we have $\langle A_i \rangle = \langle B_j \rangle = 1/2$, otherwise it is biased. A remarkable result implied by this theorem is that the recognition and optimization problems for correlation functions and unbiased quantum correlation vectors

can be solved in polynomial time by semidefinite programming (SDP). Using the theorem, we can verify that (3) is a quantum correlation vector by exhibiting the vectors:

$$u^{1} = (\frac{1}{2}, 0, \frac{1}{2}), \quad u^{2} = (0, \frac{1}{2}, \frac{1}{2}),$$

$$v^{1} = (\frac{-1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}, \frac{1}{2}), \quad v^{2} = (\frac{1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}, \frac{1}{2}).$$
(5)

Furthermore, it can be verified by SDP that this is the maximum violation of (2), although in this case Tsirelson [5] has provided an analytic proof. These maximum quantum violations have many interesting applications, see e.g. [7]. The maximum quantum violation of any Bell inequality (like CHSH) that does not have terms involving the expectations $\langle A_i \rangle$ or $\langle B_j \rangle$ can likewise be found by using SDP. Unfortunately, most of the Bell inequalities produced recently [1] do not satisfy these conditions. For these inequalities the maximum quantum violation may only be achieved by a biased quantum correlation vector, and the above method cannot be directly applied.

Tsirelson's theorem may not hold for experimental outcomes that are biased. Consider the outcome for m=n=1 given by x=(3/4,3/4,3/4). If we set $u^1=(\sqrt{3}/4,3/4)$ and $v^1=(-\sqrt{3}/4,3/4)$ then

$$x_1 = ||u^i||, \quad x_2 = ||v^1||, \quad x_{12} = ||u^1 - v^1||,$$

and the corresponding vector y=(3/4) is obviously a quantum correlation function. However x is not a quantum correlation vector because it violates the no-signalling condition. This condition derives from the fact that the expectations $\langle A_i \rangle$, $1 \leq i \leq m$ should be the same regardless of which measurement j the other party decides to make, due to the spatial separation of the two parties. Similar conditions should hold for the expectations $\langle B_j \rangle$. It is shown in [2] that a vector x satisfies the no-signalling condition if and only if it belongs to the rooted semimetric polytope defined by the inequalities:

$$x_i + x_j + x_{ij} \le 2, \quad x_i + x_j - x_{ij} \ge 0,$$

 $x_i - x_j + x_{ij} \ge 0, \quad -x_i + x_j + x_{ij} \ge 0.$ (6)

It is easy to see that unbiased quantum correlation vectors satisfy the no-signalling condition. However, the vector x = (3/4, 3/4, 3/4) violates the first of these inequalities.

It is tempting to conjecture that an outcome x is a quantum correlation vector if it satisfies the no-signalling conditions (6) and the corresponding vector y is a quantum correlation function. However, consider the vectors

$$x = \left(\frac{1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}, \frac{1}{2}, \frac{1}{2}, \frac{2+\sqrt{2}}{4}, \frac{2-\sqrt{2}}{4}, \frac{2-\sqrt{2}}{4}, \frac{2-\sqrt{2}}{4}\right)$$
$$y = \left(\frac{2+\sqrt{2}}{4}, \frac{2-\sqrt{2}}{4}, \frac{2-\sqrt{2}}{4}, \frac{2-\sqrt{2}}{4}\right).$$

The outcome x satisfies (6), and y is a quantum correlation function, as shown by the vectors given in (5). Nevertheless, it is proved in [3] that x is not a quantum correlation vector. Perhaps even more surprising is a non-quantum outcome they exhibit for the case m = n = 3:

$$x_i = \frac{1}{3}$$
, $1 \le i \le 6$, $x_{11} = x_{22} = 0$, $x_{ij} = \frac{2}{3}$
for all other $1 \le i < j \le 3$.

This gives an outcome x which satisfies (6) and for which the corresponding correlation function can even be obtained classically. For example with vectors

$$u^{1} = v^{1} = (0, 0, 0, 1/3), \quad u^{2} = v^{2} = (0, 0, 1/3, 0),$$

 $u^{3} = (1/3, 0, 0, 0), \quad v^{3} = (0, 1/3, 0, 0)$

we have

$$x_{ij} = ||u^i - v^j||_1 \quad 1 \le i < j \le 3.$$

and can use the L_1 characterization theorem given in the previous section.

Even though Tsirelson's theorem does not give a characterization of quantum correlation vectors, it can be extended to give a necessary condition that can be combined with the no-signalling condition.

Necessary conditions for quantum correlation vectors [2].

If $x = (\langle A_i \rangle, \langle B_j \rangle, \langle A_i \triangle B_j \rangle) \in [0, 1]^M$ is a quantum correlation vector then

- x must satisfy the no-signalling conditions (6), and
- There exist vectors $u^i, v^j \in \mathbb{R}^d$, $1 \le i \le m$, $1 \le j \le n$, $d \le m+n$, for which

$$x_i = ||u^i||, \quad x_{m+j} = ||v^j||, \quad x_{ij} = ||u^i - v^j||.$$

where $||u|| \equiv u^T u$.

Using this theorem, it can be shown that in the two previous examples the outcomes are not quantum correlation vectors. It also provides an efficient means of bounding the maximum quantum violation of general Bell inequalities by semidefinite programming (SDP). The strength of the no-signalling conditions with respect to various known Bell inequalities is discussed further in C.

It has recently been shown that the above conditions are not sufficient: in Doherty et al. [11] and Navascués et al. [21] a hierarchy of SDPs is presented which in some cases gives much tighter bounds. A characterization of quantum correlation vectors is given by an infinite hierarchy of conditions, each of which can be tested by solving an SDP. This work is reviewed in Section 8. It is still, however, an open problem to determine whether or not there is a polynomial time algorithm to determine whether a given vector is a quantum correlation vector.

4 A proof of Tsirelson's theorem

In this section we give an elementary description of the easy direction in Tsirelson's proof. For the proof, it is convenient to let the observables $A_1, ..., A_m, B_1, ..., B_n$ take values ± 1 rather than 0/1, and to consider the products $\langle A_i B_j \rangle$ rather than the differences $\langle A_i \triangle B_j \rangle$. An outcome is now given by

$$x = (\langle A_i \rangle, \langle B_j \rangle, \langle A_i B_j \rangle)$$

$$\equiv (\langle A_i \rangle_{1 \le i \le m}, \langle B_j \rangle_{1 \le j \le n}, \langle A_i B_j \rangle_{1 \le i \le m, 1 \le j \le n}),$$

and is called a quantum correlation vector if it can result from a quantum experiment. Similarly we redefine a quantum correlation function. In this section we use the ket-bra notation

where $|u\rangle$ denotes a (possibly complex) vector, $\langle u|$ denotes the transpose of its complex conjugate, and $\langle u|v\rangle$ denotes inner product. Using these new notations, the theorem takes the following equivalent form [5, 27].

Theorem 1 (Tsirelson's Theorem (±1 version)) For real $m \times n$ matrix c_{ij} , the followings are equivalent:

- (1) $y = (c_{ij}) \in [-1, 1]^{mn}$ is a quantum correlation function.
- (2) $x = (0,0,...,0,c_{ij}) \in [-1,1]^{m+n+mn}$ is a quantum correlation vector.
- (3) There exist two sets of unit vectors $\{u^i\}_{i=1}^m, \{v^j\}_{j=1}^n \in \mathbb{R}^d, d \leq m+n, \text{ for which } \{u^i\}_{i=1}^m, \{v^j\}_{j=1}^n \in \mathbb{R}^d, d \leq m+n, \text{ for which } \{u^i\}_{i=1}^m, \{v^j\}_{j=1}^n \in \mathbb{R}^d, d \leq m+n, \text{ for which } \{u^i\}_{i=1}^m, \{v^j\}_{j=1}^n \in \mathbb{R}^d, d \leq m+n, \text{ for which } \{u^i\}_{i=1}^m, \{v^j\}_{j=1}^n \in \mathbb{R}^d, d \leq m+n, \text{ for which } \{u^i\}_{i=1}^m, \{v^j\}_{j=1}^n \in \mathbb{R}^d, d \leq m+n, \text{ for which } \{u^i\}_{i=1}^m, \{u^i\}$

$$c_{ij} = \langle u^i | v^j \rangle$$
.

(4) There exist two sets of vectors $\{u^i\}_{i=1}^m$ and $\{v^j\}_{j=1}^n$ on $\mathbb{R}^{\min(m,n)}$ such that they satisfy $|u^i| \leq 1$, $|v^j| \leq 1$ for all i and j,

$$c_{ij} = \langle u^i | v^j \rangle \,. \tag{7}$$

(5) There exist a state on a composite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ and two sets of Hermitian operator $\{A_i\}_{i=1}^m$ on a Hilbert space \mathcal{H}_A and $\{B_j\}_{j=1}^n$ on a Hilbert space \mathcal{H}_B such that $|A_i| \leq I$, $|B_j| \leq I$, and

$$c_{ij} = \operatorname{Tr}(A_i \otimes B_j \rho). \tag{8}$$

Proof: If (1) holds, some quantum correlation vector x' must be consistent with y. By switching the outcomes +1 and -1 we see that the vector x'' formed by setting $x_i'' = -x_i'$, i = 1, ..., m + n and otherwise setting $x_{ij}'' = x_{ij}'$ is also a quantum correlation vector. The implication $(1) \Rightarrow (2)$ then follows from the convexity of the set of quantum correlation vectors by setting x = (x' + x'')/2.

The implication $(2) \Rightarrow (3)$ follows from the postulates of quantum theory. Indeed, corresponding to the given quantum correlation vector there must exist observables $A_1, ..., A_m$ on a Hilbert space \mathcal{H}_A , observables $B_1, ..., B_n$ on a Hilbert space \mathcal{H}_B , and a pure quantum state $|\psi\rangle$ given as a unit vector on $\mathcal{H}_A \otimes \mathcal{H}_B$, where \otimes denotes tensor (Kronecker) product. For $1 \leq i \leq m$ and $1 \leq j \leq n$, let $|a^i\rangle = A_i \otimes I_B |\psi\rangle$ and $|b^j\rangle = I_A \otimes B_j |\psi\rangle$. Then $|a^i\rangle$ and $|b^j\rangle$ are (possibly complex) unit vectors of length, say, t, such that $\langle a^i|b^j\rangle = \langle A_iB_j\rangle$. We may replace them with real vectors u^i and v^j of length 2t by writing the real and complex coefficients as separate coordinates, maintaining the same values of the inner products. The set of m+n real vectors $u^1, ..., u^m, v^1, ..., v^n$ have all the properties of part (2) except possibly their dimension 2t > m+n. However the unit vectors lie in a subspace of dimension $d \leq m+n$, which preserves their inner products. We can also prove $(5) \Rightarrow (4)$ in the same way.

Now, we prove $(4) \Rightarrow (5)$ and $(3) \Rightarrow (1)$. Suppose the condition (4) (or the condition (3)) holds, and $\xi = \min\left(\dim \operatorname{span}\{u^i\}_i^m, \dim \operatorname{span}\{v^j\}_j^n\right)$ (or $\xi = d$ for the condition (3)). We choose a Hilbert space \mathcal{H} whose dimension is 2^{ν} , where $\nu = \frac{\xi}{2}$ for even ξ , and $\nu = \frac{\xi-1}{2}$ for odd ξ . Then, there exists an irreducible representation of the Clifford algebra on \mathcal{H} , and we can choose a set of ξ Hermitian operators $\{X_k\}_{k=1}^{\xi}$ as an irreducible representation of a generator set of the Clifford algebra (see A); that is, $\{X_k\}_{k=1}^{\xi}$ satisfies the following anti-commutation relation:

$$X_i X_j + X_j X_i = 2\delta_{ij} I. (9)$$

Then, from the above relation, Hermitian operators $\{X_k \otimes X_k\}_{k=1}^{\xi}$ commute with each other. Thus, they have simultaneous eigenvectors, and moreover, their corresponding eigenvalues are ± 1 . Therefore, there exists a state $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ which is a simultaneous eigenvector of $\{X_k \otimes X_k\}_{k=1}^{\xi}$ satisfying

$$X_k \otimes X_k |\Psi\rangle = (-1)^{a_k} |\Psi\rangle \tag{10}$$

where a_k is 0 or 1. Then, $|\Psi\rangle$ and $\{X_k\}_{k=1}^{\xi}$ satisfies

$$\langle \Psi | X_k \otimes X_l | \Psi \rangle$$

$$= \frac{1}{2} \{ (-1)^{a_l} \langle \Psi | X_k X_l \otimes I | \Psi \rangle$$

$$+ (-1)^{a_l} \langle \Psi | X_l X_k \otimes I | \Psi \rangle \}$$

$$= \frac{1}{2} (-1)^{a_l} \langle \Psi | (X_k X_l + X_l X_k) \otimes I | \Psi \rangle$$

$$= (-1)^{a_l} \delta_{kl} I, \tag{11}$$

where we use Eq.(10) in the first equality and Eq.(9) in the third equality. Finally, we define A_i and B_j as

$$A_{i} = \sum_{k=1}^{\xi} (u'^{i})_{k} X_{k}$$

$$B_{j} = \sum_{k=1}^{\xi} (-1)^{a_{k}} (v'^{j})_{k} X_{k},$$
(12)

where u'^i and v'^j are vectors derived by projecting u^i and v^j onto span $\{u^i\}_{i=1}^m$ in the case of dim span $\{u^i\}_{i=1}^m \leq \dim \operatorname{span}\{v^j\}_{j=1}^n$ and onto span $\{v^j\}_{j=1}^m$ otherwise (for condition (3), we can just choose $u'^i = u^i$ and $v'^i = v^i$). By their definition, we can easily see that $A_i^2 = |u'^i|^2 I$ and $B_j^2 = |v'^j|^2 I$. This fact guarantees that $|A_i| \leq I$ and $|B_j| \leq I$ (for the condition (3), A_i and B_j take eigenvalues ± 1). Finally, we can calculate $\langle \Psi | A_k \otimes B_l | \Psi \rangle$ as follows:

$$\langle \Psi | A_i \otimes B_j | \Psi \rangle$$

$$= \sum_{kl} (-1)^{a_l} (u'^i)_k (v'^j)_l \langle \Psi | X_k \otimes X_l | \Psi \rangle$$

$$= \sum_{kl} (-1)^{2a_l} (u'^i)_k (v'^j)_l \delta_{kl}$$

$$= \langle u'^i | v'^j \rangle$$

$$= \langle u^i | v^j \rangle$$
(13)

where we use Eq.(11) in the second equality.

In the above proof of $(4) \Rightarrow (5)$ and $(3) \Rightarrow (1)$, in order to satisfy the equation $\langle \Psi | A_i \otimes B_j | \Psi \rangle = \langle u^i | v^j \rangle$, Tsirelson used the simultaneous eigenvector $|\Psi\rangle$ corresponding to eigenvalue "1" of $\{X_k\}_{k=1}^{\xi}$ [26]. With A_i and B_j defined by Eq.(12) and $a^k = 0$, we showed that we can choose an arbitrary simultaneous eigenvector of $\{X_k \otimes X_k\}_{k=1}^{\xi}$ by slightly changing the definition of A_i and B_j from Tsirelson's original definition. As we will see later, this modification of the proof is actually important for finding an explicit optimal construction of A_i and B_j .

5 Representing two dimensional vectors

In order to illustrate the concepts, we give a construction of a quantum setting that can realize the inner products of two dimensional vectors. Let $u^1, ..., u^m$ and $v^1, ..., v^n$ be m+n unit vectors in \mathbb{R}^2 and let $z=(z_1,z_2)$. Define

$$C(z) = \left[\begin{array}{cc} z_1 & z_2 \\ z_2 & -z_1 \end{array} \right].$$

Now define observables

$$A_i = C(u^i), \quad B_i = C(v^j), \quad i = 1, ..., m \quad j = 1, ..., n.$$

Let $|\Psi\rangle = [1/\sqrt{2}, \ 0, \ 0, \ 1/\sqrt{2}]^T$ which corresponds to the state $\frac{|00\rangle + |11\rangle}{\sqrt{2}}$. Then it is easy to verify that Eq.(13) holds. For example, with

$$u^{1} = [1, 0]^{T}, \quad u^{2} = [0, 1]^{T},$$

 $v^{1} = [1/\sqrt{2}, 1/\sqrt{2}]^{T}, \quad v^{2} = [1/\sqrt{2}, -1/\sqrt{2}]^{T}$

we may verify, for instance, that

$$\langle u^2|v^1\rangle = \langle \Psi|C(u^2)\otimes C(v^1)|\Psi\rangle = \frac{1}{\sqrt{2}}.$$

Incidentally, this gives a quantum setting for the maximum violation of the CHSH inequality described in Section 2, when the inequality is restated in ± 1 terms.

Here is how the quantum setting is obtained. We start with

$$X_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
 $X_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

It is easy to verify that the anti-commutation relation (9) holds (that is, X_1, X_2 are a representation of the generators of the Clifford algebra $Cl(\mathbb{R}^2)$) and that C(z) = X(z) as given by (12) with $a_k = 0$. To get the state $|\Psi\rangle$ we first construct the operator A given by

$$2A = X_1 \otimes X_1 + X_2 \otimes X_2 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}.$$

Using Maple we find that A has maximum eigenvalue 1 with corresponding eigenvector $[1, 0, 0, 1]^T$. When normalized, this eigenvector gives the state $|\Psi\rangle$ above.

6 Construction of a state and observables which represent correlation functions

In this section, we give a general construction, that is, states and operators which can represent all correlation functions. By using the theory of stabilizer states, especially, the binary representation of stabilizer formalism, we show that we can always choose a standard singlet for a state to represent all correlation functions. We believe this is the first time an explicit construction has been given. For the convenience of readers, we give a review of the binary representation of stabilizer formalism in B.

We are interested in the construction of the states $|\Psi\rangle$ and observables A_i and B_j satisfying $|A_i| \leq I$, $|B_j| \leq I$ (or $|A_i| = |B_j| = I$), and

$$\langle \Psi | A_i \otimes B_j | \Psi \rangle = \langle u^i | v^j \rangle \tag{14}$$

in the case when two sets of vectors $\{u^i\}_{i=1}^m$ and $\{v^j\}_{j=1}^n$ satisfying the fourth condition (or the third condition) of Theorem 1 are given. As we have seen in the proof of the theorem, suppose $\xi = \min\left(\dim \operatorname{span}\{u^i\}_i^m, \dim \operatorname{span}\{v^j\}_j^n\right)$ for the fourth condition, and $\xi = d$ for the third condition. Then, these vectors are represented in a Hilbert space \mathcal{H} whose dimension is 2^{ν} ($\nu = \frac{\xi}{2}$ for even ξ , and $\nu = \frac{\xi-1}{2}$ for odd ξ) as Eq.(12) by using a representation of the generators of the Clifford algebra $\{X_k\}_{k=1}^{\xi}$ and their simultaneous eigenvector $|\Psi\rangle$. Therefore, in order to construct $|\Psi\rangle$, A_i and B_j , we need to know how we can find a simultaneous eigenvector $|\Psi\rangle$ corresponding to $\{X_k\}_{k=1}^{\xi}$. In what follows, we give an explicit way to do it.

First, we consider the case when ξ is even; that is, $\xi = 2\nu$; In this case, we can choose the Weyl-Brauer matrices as an irreducible representation of the generators of the Clifford algebra on \mathcal{H}_A and \mathcal{H}_B as follows (see A):

$$X_{k} \stackrel{\text{def}}{=} \underbrace{Z \otimes \cdots \otimes Z}_{k-1} \otimes X \otimes \underbrace{I \otimes \cdots \otimes I}_{\nu-k},$$

$$X_{k+\nu} \stackrel{\text{def}}{=} -\underbrace{Z \otimes \cdots \otimes Z}_{k-1} \otimes Y \otimes \underbrace{I \otimes \cdots \otimes I}_{\nu-k},$$

$$(15)$$

where X, Y and Z are the Pauli matrices, and an index k satisfies $1 \leq k \leq \nu$ [30]. Since $\{X_k\}_{k=1}^{2\nu}$ is a set of Hermitian operators which are composed of tensor products of Pauli operators satisfying Eq.(9), $\{X_k \otimes X_k\}_{k=1}^{2\nu}$ generate a commutable subgroup of the Pauli Group [15, 28, 17] on 2ν qubits $\mathcal{P}_{2\nu}$; we write this commutable subgroup as $S_{2\nu}$. Note that Eq.(15) guarantees independence of the generator $\{X_k \otimes X_k\}_{i=1}^{2\nu}$. Since $|\Psi\rangle$ is defined as the simultaneous eigenvector of $\{X_k \otimes X_k\}_{k=1}^{2\nu}$ corresponding to an eigenvalue 1 for all $X_k \otimes X_k$, $|\Psi\rangle$ is nothing but a stabilizer state corresponding to the independent and commutative Pauli group elements $\{X_k \otimes X_k\}$. Here, in a n-qubit Hilbert space, a stabilizer state $|\Psi\rangle$ of commutative and independent Pauli group elements $\{M_k\}_{k=1}^n$ is defined as a state which satisfies $M_i |\Psi\rangle = |\Psi\rangle$ for all i [28, 17]. In this case, a set of 2^n commuting Pauli operators $S \stackrel{\text{def}}{=} \{M \in \mathcal{P}_n | M |\Psi\rangle = |\Psi\rangle\}$ is called a stabilizer group of the state $|\Psi\rangle$; thus, $\{M_k\}_{k=1}^n$ are independent generators of the commutative group S. Conversely, a set of S commuting Pauli operators all of which have real overall phase S uniquely define a corresponding stabilizer state by the equations S is S for all S or S and S is the final a concrete expression for a stabilizer state S or S or S is all S or S or S in S or S in S in S or S in S in

is generated by $\{X_k \otimes X_k\}_{k=1}^{\xi}$. For the case when $\xi = 2\nu + 1$, we can choose an irreducible representation of the generators of the Clifford algebra on $\mathcal{H}_A \otimes \mathcal{H}_B$ as $\{X_k\}_{k=1}^{2\nu+1}$ where $\{X_k\}_{k=1}^{2\nu}$ are defined by Eq.(15)

and $X_{2\nu+1} \stackrel{\text{def}}{=} \overbrace{Z \otimes \cdots \otimes Z}^{\nu}$ (see A). Since the equality $X_{2\nu+1} = (-i)^{\nu} \Pi_{k=1}^{2\nu} X_k$ holds, we derive the equality $X_{2\nu+1} \otimes X_{2\nu+1} = (-1)^{\nu} \Pi_{k=1}^{2\nu} X_k \otimes X_k \in S_{2\nu}$. Thus, a stabilizer state $|\Psi\rangle$ of the stabilizer group $S_{2\nu}$ automatically satisfies $X_{2\nu+1} \otimes X_{2\nu+1} |\Psi\rangle = (-1)^{\nu+\sum_{k=1}^{2\nu} a_k} |\Psi\rangle$. Therefore, by defining $a_{2\nu+1} = \nu + \sum_{k=1}^{2\nu} a_k$, the state $|\Psi\rangle$ is nothing but the state which satisfies $\langle \Psi | A_i \otimes B_j | \Psi \rangle = \langle u^i | v^j \rangle$ for A_i and B_j defined by Eq.(12).

So far, we showed that the state $|\Psi\rangle$ satisfying Eq.(14) is a stabilizer state of the group $S_{2\nu}$ which is generated by $\{X_k \otimes X_k\}_{k=1}^{2\nu}$. In order to construct a simultaneous eigenstate of $\{X_k \otimes X_k\}_{k=1}^{2\nu}$ defined by Eq.(15), we find a graph state which is equivalent to $|\Psi\rangle$ under local Clifford operations by using the binary representation of the stabilizer formalism, which was mainly developed in [15] and [28] (See B). Here, a graph state is a state in the standard form of stabilizer states [17], and defined by means of an n-vertex graph G with adjacency matrix $\{\theta_{ij}\}_{ij}$ as the stabilizer state generated by commuting Pauli's operators $\{K_j\}_{j=1}^n$ defined as

$$K_j = X^{(j)} \Pi_{k=1}^n \left(Z^{(k)} \right)^{\theta_{kj}}. \tag{16}$$

Here $X^{(i)}$ and $Z^{(i)}$ are the Pauli operators having X and Z in the ith position of the tensor product and the identity elsewhere, respectively. We note that the binary generator matrix K corresponding to $\{K_j\}_{j=1}^n$ can be written as the following simple form:

$$K = \stackrel{\text{def}}{=} \left[\begin{array}{c} \theta \\ I \end{array} \right]. \tag{17}$$

In the binary representation, the set of Pauli operators $\{X_k \otimes X_k\}_{k=1}^{2\nu}$ defined in Eq.(15) is written as

$$X_{k} \otimes X_{k} \leftrightarrow \underbrace{(1 \cdots 1 0 \cdots 0 \mid 1 \cdots 1 0 \cdots 0 \mid}_{k-1} \underbrace{(1 \cdots 1 0 \cdots 0 \mid 1 \cdots 1 0 \cdots 0 \mid}_{0 \cdots 0 \mid 1 0 \cdots 0 \mid 1 0 \cdots 0}]^{\nu-k+1}$$

$$X_{k+\nu} \otimes X_{k+\nu} \leftrightarrow \underbrace{(1 \cdots 1 0 \cdots 0 \mid 1 \cdots 1 0 \cdots 0 \mid}_{k-1} \underbrace{(1 \cdots 1 0 \cdots 0 \mid 1 \cdots 1 0 \cdots 0 \mid}_{0 \cdots 0 \mid 1 0 \cdots 0 \mid 1 0 \cdots 0}]^{\nu-k}$$

where $1 \le k \le \nu$. The generator matrix E corresponding to a set of Pauli operators $\{X_k \otimes X_k\}_{k=1}^{2\nu}$ can be written as

$$E \stackrel{\text{def}}{=} \begin{pmatrix} T_{\nu-1} & T_{\nu} \\ T_{\nu-1} & T_{\nu} \\ I & I \\ I & I \end{pmatrix}, \tag{18}$$

where $T_{\nu-1}$ and T_{ν} are $\nu \times \nu$ matrices defined as

$$T_{
u-1} \stackrel{\mathrm{def}}{=} \left(egin{array}{cccc} 0 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 1 & \cdots & 1 \\ dots & \ddots & \ddots & \ddots & dots \\ 0 & 0 & & 0 & 1 \\ 0 & 0 & & \cdots & 0 \end{array}
ight),$$
 $T_{
u} \stackrel{\mathrm{def}}{=} \left(egin{array}{cccc} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & 1 \\ \ddots & \ddots & \ddots & dots \\ 0 & & 0 & 1 \end{array}
ight),$

and I is a $\nu \times \nu$ identity matrix.

In order to find a graph state which is equivalent to $|\Psi\rangle$ under local Clifford operations, we try to transform the above generator matrix E into the form of Eq.(17), which corresponds to a generator matrix of graph states, by changing the basis of the stabilizer and using local Clifford operations. As we can see in B, a change of the basis of a stabilizer corresponds to applying an invertible matrix from the right-hand side of E, and an application of local Clifford operations to the state $|\Psi\rangle$ is equivalent to applying a symplectic matrix from the left-hand side of E. Following a discussion which is similar to that used in [28], we can find and easily check the following equation:

$$L \cdot E \cdot R_1 \cdot R_2 = F,\tag{19}$$

where L, R_1 , R_2 , F are defined as

$$L \stackrel{\text{def}}{=} \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & 0 & I \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \end{bmatrix}, \quad R_1 \stackrel{\text{def}}{=} \begin{bmatrix} T_{\nu-1} & T_{\nu} \\ T_{\nu-1} & T_{\nu} \\ I & I \end{bmatrix},$$

$$R_2 \stackrel{\text{def}}{=} \begin{bmatrix} I & T_{\nu} \\ T_{\nu} & I \end{bmatrix}, \quad F \stackrel{\text{def}}{=} \begin{bmatrix} 0 & I \\ I & 0 \\ I & 0 \\ 0 & I \end{bmatrix}. \tag{20}$$

We also easily see that L is symplectic, R_1 and R_2 are invertible, and F is in the form of Eq.(17); that is, F is a generator matrix corresponding to a graph state. Actually, in comparison with Eq.(17), in this case, the adjacency matrix of the graph state corresponding to F is $\theta = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}$. A way of constructing an arbitrary graph state is already known [17]. Thus, we can easily see the graph state $|\Psi'\rangle$ corresponding to F is

$$|\Psi'\rangle = \bigotimes_{k=1}^{\nu} \frac{1}{\sqrt{2}} \left(|+0\rangle_{A_k B_k} \otimes |-1\rangle_{A_k B_k} \right), \tag{21}$$

where $|+\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$ and $|-\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$ and that $|\Psi'\rangle$ is equivalent to n singlets. As we can see in B, in Eq.(19), applying R_1 and R_2 corresponds to changing the generators of a stabilizer group of $|\Psi\rangle$, and applying L actually corresponds to applying a Clifford operation on $|\Psi\rangle$. As we can easily check, a binary symplectic matrix L corresponds to a "local" Clifford operation $\mathcal{L} \stackrel{\text{def}}{=} I \otimes \cdots \otimes I \otimes H \otimes \cdots \otimes H$, where the first n-qubits belong to \mathcal{H}_A , the next n-qubits belong to \mathcal{H}_B , and H is a Hardmer operator. Thus, the stabilizer groups corresponding to $|\Psi\rangle$ and $\mathcal{L}^{\dagger} |\Psi'\rangle = \mathcal{L} |\Psi'\rangle$ have the same binary representation $E = L^{-1} \cdot F \cdot R_2^{-1} \cdot R_1^{-1}$. This fact does not guarantee $|\Psi\rangle = \mathcal{L} |\Psi'\rangle$. However, this fact guarantees that $\mathcal{L} |\Psi'\rangle$ is a simultaneous eigenvector of $\{X_k \otimes X_k\}_{k=1}^{2\nu}$, which is a stabilizer of $|\Psi\rangle$. In fact, we can easily check that $\mathcal{L} |\Psi'\rangle = \bigotimes_{i=1}^{\nu} \frac{1}{\sqrt{2}} (|++\rangle + |--\rangle)$ satisfies the following equations: For $1 \leq k \leq \nu$,

$$X_{k} \otimes X_{k} \mathcal{L} | \Psi' \rangle = \mathcal{L} | \Psi' \rangle$$

$$X_{k+\nu} \otimes X_{k+\nu} \mathcal{L} | \Psi' \rangle = -\mathcal{L} | \Psi' \rangle$$

$$X_{2\nu+1} \otimes X_{2\nu+1} \mathcal{L} | \Psi' \rangle = \mathcal{L} | \Psi' \rangle,$$

where we only use $X_{2\nu+1}$ in the case ξ is odd. Therefore, as we have already mentioned, we can set $a_k = 0$ for $1 \le k \le \nu$ and $k = 2\nu + 1$, and $a_k = 1$ for $\nu + 1 \le k \le 2\nu$, and we also define A_i and B_j by Eq.(12). Then, $|\Psi''\rangle \stackrel{\text{def}}{=} \mathcal{L} |\Psi'\rangle$ satisfies

$$\langle \Psi'' | A_i \otimes B_j | \Psi'' \rangle = \langle u^i | v^j \rangle. \tag{22}$$

Finally, as a result, by applying $H \otimes \cdots \otimes H$ to both $|\Psi''\rangle$ and $\{X_k \otimes X_k\}_{k=1}^{2\nu+1}$, we derive the following Theorem.

Theorem 2 Given vectors $\{u^i\}_{i=1}^m$ and $\{v^j\}_{j=1}^n$ on $\mathbb{R}^{\min(m,n)}$ satisfying $|u^i| \leq 1$, $|v^j| \leq 1$ for all i and j, there are operators $\{A_i\}_{i=1}^m$ and $\{B_j\}_{j=1}^n$ on 2ν qubits which satisfy $|A_i| \leq I$, $|B_j| \leq I$, and

$$\langle \Phi_+ |^{\otimes \nu} A_i \otimes B_j | \Phi_+ \rangle^{\otimes \nu} = \langle u^i | v^j \rangle,$$
 (23)

where $|\Phi_{+}\rangle \stackrel{\text{def}}{=} |00\rangle + |11\rangle$, $\nu = \lfloor \frac{\xi}{2} \rfloor$, $\xi = \min \left(\dim \operatorname{span}\{u^{i}\}_{i}^{m}, \dim \operatorname{span}\{v^{j}\}_{j}^{n} \right)$, and A_{i} and B_{j} are defined as

$$A_{i} = \sum_{k=1}^{\xi} (u'^{i})_{k} X_{k}$$

$$B_{j} = \sum_{k=1}^{\xi} (-1)^{a_{k}} (v'^{j})_{k} X_{k}.$$

In the above, u'^i and v'^j are vectors derived by projecting u^i and v^j onto $\operatorname{span}\{u^i\}_{i=1}^m$ in the case of $\dim \operatorname{span}\{u^i\}_{i=1}^m \leq \dim \operatorname{span}\{v^j\}_{j=1}^n$ and onto $\operatorname{span}\{v^j\}_{j=1}^m$ otherwise,

$$X_{k} \stackrel{\text{def}}{=} \overbrace{X \otimes \cdots \otimes X}^{k-1} \otimes Z \otimes \overbrace{I \otimes \cdots \otimes I}^{\nu-k} \quad (1 \leq k \leq \nu)$$

$$X_{k+\nu} \stackrel{\text{def}}{=} \overbrace{X \otimes \cdots \otimes X}^{\nu} \otimes Y \otimes \overbrace{I \otimes \cdots \otimes I}^{\nu-i} \quad (1 \leq k \leq \nu)$$

$$X_{2\nu+1} \stackrel{\text{def}}{=} \overbrace{X \otimes \cdots \otimes X}^{\nu}$$

and

$$a_k = 0 \ (1 \le k \le \nu \text{ and } k = 2\nu + 1)$$

 $a_k = 1 \ (\nu + 1 \le k \le 2\nu).$

That is, by choosing observables as above, n copies of a standard 2-dimensional maximally entangled state gives a quantum correlation which is represented by a correlation function $\langle u^i|v^j\rangle$. Although we used the fourth condition of Tsirelson's theorem (Theorem 1) in the above theorem, we can also use the third condition of the theorem. In this case, we just need to modify ξ as $\xi=d$ instead.

7 Optimality of the construction

As we can easily see from the discussion in the previous section, by choosing observables appropriately, the state $|\Phi_+\rangle^{\otimes \nu}$ actually gives any quantum correlation function $c_{ij} = \langle u^i | v^j \rangle$

satisfying $\xi \leq 2\nu + 1$, where $\xi \stackrel{\text{def}}{=} \min \left(\dim \operatorname{span}\{u^i\}_i^m, \dim \operatorname{span}\{v^j\}_j^n \right)$. Moreover, when a quantum correlation function c_{ij} is an extremal point of the set of all $m \times n$ quantum correlation functions, this choice of a state and observables is actually the unique optimal choice with respect to both the dimension of the Hilbert space and the amount of entanglement, up to local unitary equivalence. This fact was also proved by Tsirelson [27]. Before we state his theorem, we should note one important fact. For an extremal c_{ij} , ξ is uniquely determined, and called the rank of c_{ij} [27]. That is, $c_{ij} = \langle u^i | v^j \rangle = \langle u'^i | v'^j \rangle$ implies $\xi = \xi'$ in this case. Here, we just give the theorem, when the rank ξ is even. The proof is found in [27].

Theorem 3 (Tsirelson) Let c_{ij} be an extremal point, with even rank ξ , of the set of all $m \times n$ quantum correlation functions. Suppose a state ρ and observables $\{A_i\}_{i=1}^m, \{B_j\}_{j=1}^n$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ satisfy Eq.(8). Then, \mathcal{H}_A and \mathcal{H}_B can be decomposed as $\mathcal{H}_A = \bigoplus_{\alpha=1}^{L+1} \mathcal{H}_{A_\alpha}$ and $\mathcal{H}_B = \bigoplus_{\beta=1}^{L+1} \mathcal{H}_{B_\beta}$ such that dim $\mathcal{H}_{A_\alpha} = \dim \mathcal{H}_{B_\beta} = 2^{\xi/2}$ for $1 \le \alpha \le L$ and $1 \le \beta \le L$. In this decomposition of the space, A_i and B_j can be written as

$$A_{i} = \left(\bigoplus_{\alpha=1}^{L} A_{i}^{(\alpha)}\right) \oplus I_{L+1}$$

$$B_{j} = \left(\bigoplus_{\beta=1}^{L} B_{j}^{(\beta)}\right) \oplus I_{L+1}, \tag{24}$$

and ρ can be written as

$$\rho = \sum_{\alpha=1}^{L} \lambda_{\alpha} |\Phi_{\alpha}\rangle \langle \Phi_{\alpha}|, \qquad (25)$$

where $\{\lambda_{\alpha}\}_{\alpha=1}^{L}$ is a probability distribution, and $|\Phi_{\alpha}\rangle\langle\Phi_{\alpha}|$ is supported by $\mathcal{H}_{A_{\alpha}}\otimes\mathcal{H}_{B_{\alpha}}$. Moreover, the state $|\Phi_{\alpha}\rangle$ and observables $\{A_{i}^{\alpha}\}_{i=1}^{m}$ and $\{B_{j}^{\alpha}\}_{j=1}^{m}$ on $\mathcal{H}_{A_{\alpha}}\otimes\mathcal{H}_{B_{\alpha}}$ is local unitary equivalent to the state $|\Phi\rangle^{\otimes\xi/2}$ and observables $\{A_{i}\}_{i=1}^{m}$ and $\{B_{j}\}_{j=1}^{m}$ defined in Theorem 2 which corresponds to the same quantum correlation function c_{ij} .

Thus, the construction given in Theorem 2 is optimal with respect to the dimension of the Hilbert space. For odd ξ , the corresponding theorem is slightly more complicated. However, the construction given in Theorem 2 is optimal also in this case [27]. Here, we note one more important fact which we can observe immediately from the above theorem. Since the observables $\{A_i\}_{i=1}^m$ and $\{B_j\}_{j=1}^n$ defined by Eq.(24) obey the anti-commutation relation, they are actually proportional to a complex representation of the generators of the Clifford algebra $Cl(\mathbb{R}^{\xi})$. Thus, a set of observables corresponding to an extremal quantum correlation function always has the structure of a Clifford algebra. Therefore, the construction using an irreducible representation of the Clifford algebra is optimal.

We can easily calculate the value of entanglement measures for the state ρ defined by Eq. (25). (The reader unfamiliar with entanglement measures is referred to [23].) First, since we can deterministically derive $|\Phi_+\rangle^{\otimes \xi/2}$ by applying projective measurement to distinguish $\{\mathcal{H}_{A_{\alpha}}\}_{\alpha=1}^{L+1}$, we derive a lower bound on the value of the distillable entanglement of $E_D(\rho) \geq \xi/2$. Second, since Eq. (25) gives a pure-states-decomposition of ρ , we derive an upper bound on the entanglement formation $E_F(\rho) \leq \xi/2$. Moreover, since ρ defined by Eq.(25) is maximally correlated, the entanglement formation $E_F(\rho)$ is additive for ρ and it coincides with the entanglement cost $E_C(\rho)$. Since any entanglement measure $E(\rho)$ satisfies $E_D(\rho) \leq E(\rho) \leq E_C(\rho)$, we can conclude $E(\rho) = E(|\Phi\rangle^{\otimes \xi/2}) = \xi/2$. Therefore, even if we use a mixed state ρ , we cannot reduce the amount of entanglement which is needed to represent an extremal quantum correlation function c_{ij} , and we actually need $\xi/2$ singlets to make such quantum correlation. In this sense, the construction given in Theorem 2 is an optimal construction with respect to both the dimension of the Hilbert space and the amount of entanglement.

We conclude this section with the following remark. In some cases, the quantum state constructed above may be too large for any conceivable practical implementation. However, there is a way to approximate the given correlations using a state with much smaller dimensions. This is by using the Johnson-Lindenstrauss Lemma, which we state in the form given in [9]:

Lemma 1 (Johnson-Lindenstrauss) For $\epsilon \in (0,1)$ and N a positive integer, let K be a positive integer such that

$$K \ge 4(\epsilon^2/2 - \epsilon^3/3)^{-1} log N.$$
 (26)

Then for any set V of N points in \mathbb{R}^d there is a mapping $f: \mathbb{R}^d \to \mathbb{R}^K$ such that for all $u, v \in V$,

$$(1 - \epsilon) \langle u | v \rangle \le \langle f(u) | f(v) \rangle \le (1 + \epsilon) \langle u | v \rangle. \tag{27}$$

To use this lemma, we set N = m+n, d = min(m,n), and let V be the union of the point sets $\{x_k\}_{k=1}^m$ and $\{y_l\}_{l=1}^n$ from Theorem 2. The lemma tells us that we may replace V by point sets in \mathbb{R}^K , which is a logarithmic reduction in dimension if m and n are comparable. Theorem 2 applied to these lower dimensional point sets gives a quantum setting where the number of qubits required is also reduced logarithmically, and for which the correlations can be made arbitrarily close to those desired.

8 The maximum violation of quantum correlation vectors

As we mentioned in Section 3, quantum correlation vectors are not characterized by Tsirelson's Theorem 1, which gives necessary and sufficient conditions for quantum correlation functions. We saw that the theorem gives necessary conditions for quantum correlation vectors that can be combined with the no-signalling condition. These necessary conditions enable us to bound the maximum quantum violation of (general) Bell inequalities [2]. However, it is not clear to what extent the no-signalling conditions improve the bound given by Tsirelson's theorem.

We denote the set of quantum correlation functions (resp. quantum correlation vectors) by $M_{\mathrm{QB}}(m,n)$ (resp. $\mathcal{Q}_{\mathrm{Cut}}(m,n)$) following the notation of [2]. The condition 3 of Theorem 1 (± 1 version) can be represented by the *elliptope* [10, section 28.4], which is well studied in combinatorial optimization. The elliptope $\varepsilon(G)$ of a graph G=(V,E) with n=|V| nodes is the convex body consisting of vectors $z=(z_{ij})\in\Re^E$ such that there exist unit vectors $u^i,u^j\in\Re^n$ for each node $i,j\in V$ satisfying $z_{ij}=\langle u^i|u^j\rangle$. Let $K_{m,n}$ be the complete bipartite graph with nodes $V_{m,n}=\{A_1,...,A_m,B_1,...,B_n\}$ and edges $E_{m,n}=\{A_iB_j\mid 1\leq i\leq m,1\leq j\leq n\}$. The elliptope $\varepsilon(K_{m,n})$ is the set of the vectors in $[-1,+1]^{mn}$ satisfying condition 3 of Theorem 1, that is:

$$M_{\text{OB}}(m,n) = \varepsilon(K_{m,n}). \tag{28}$$

We can apply condition 3 of Theorem 1 to quantum correlation vectors as follows:

• For a quantum correlation vector $x = (c_{kl}) \in [-1, +1]^{m+n+mn}$, there exist three sets of unit vectors $\{t^h\}_{h=1}, \{u^i\}_{i=1}^m, \{v^j\}_{j=1}^n \in \mathbb{R}^d$, and $d \leq 1 + m + n$, for which

$$x = (c_{kl})$$

$$= (\langle t^1 | u^i \rangle_{1 \le i \le m}, \langle t^1 | v^j \rangle_{1 \le j \le n},$$

$$\langle u^i | v^j \rangle_{1 < i < m, 1 < j < n}).$$

The set of the vectors satisfying the latter conditions corresponds to the elliptope of another graph $\nabla K_{m,n}$ called the suspension graph of $K_{m,n}$. The graph $\nabla K_{m,n} = (\nabla V_{m,n}, \nabla E_{m,n})$ is defined as the graph with 1+m+n nodes $\nabla V_{m,n} = \{X\} \cup V_{m,n}$ and m+n+mn edges $\nabla E_{m,n} = \{XA_i \mid 1 \leq i \leq m\} \cup \{XB_j \mid 1 \leq j \leq n\} \cup E_{m,n}$. The no-signalling conditions correspond to the rooted semimetric polytope denoted by $\mathrm{RMet}(\nabla K_{m,n})$, which has been also well studied [10, section 27.2], and is given by the following inequalities in the ± 1 version:

$$\begin{array}{rcl} x_{XA_i} + x_{XB_j} + x_{A_iB_j} & \geq & -1, \\ x_{XA_i} + x_{XB_j} - x_{A_iB_j} & \leq & 1, \\ x_{XA_i} - x_{XB_j} + x_{A_iB_j} & \leq & 1, \\ -x_{XA_i} + x_{XB_j} + x_{A_iB_j} & \leq & 1. \end{array}$$

Quantum correlation vectors are bounded as follows [2, Theorem 6]:

$$Q_{\text{Cut}}(m,n) \subseteq \varepsilon(\nabla K_{m,n}) \cap \text{RMet}(\nabla K_{m,n}). \tag{29}$$

It has recently been shown that the inclusion in equation (29) is in fact proper. Navascués, et al. [21] recently succeeded in completely characterizing the set of all quantum correlation vectors by means of a sequence of SDPs [21]. Using this characterization they got a tight upper bound on the quantum violation of the Froissart Bell inequality, I_{3322} (see [13],[8]) of .25089. This is significantly tighter than the bound of 0.3660 given by the right hand side of (29) for this inequality [2]. A similar computational result was reported by Doherty et al. [11], also using a hierarchy of SDPs. The lower bound on the quantum violation is .25 [8].

We begin by reviewing the work of Navascués, et al. First, they treat a more general problem setting. That is, their result is valid for all quantum correlation experiments which consist of measurements having any number of outcomes. So, we need to generalize the definition of a quantum correlation vector. Suppose Alice's and Bob's measurements are described by projective measurements $\{E_{\alpha}^{(i)}\}_{\alpha=1}^{a(i)}$ and $\{F_{\beta}^{(j)}\}_{\beta=1}^{b(j)}$, where a(i) and b(j) are the number of outcomes of the ith and jth measurements of Alice and Bob, respectively. That is, this set of operators satisfies

$$E_{\alpha}^{(i)} = E_{\alpha}^{(i)\dagger}, \ F_{\beta}^{(j)} = F_{\alpha}^{(j)\dagger},$$

$$\sum_{\alpha=1}^{a(i)} E_{\alpha}^{(i)} = I, \ \sum_{\beta=1}^{b(j)} F_{\beta}^{(j)} = I,$$

$$E_{\alpha}^{(i)} E_{\alpha'}^{(i)} = \delta_{\alpha\alpha'} E_{\alpha}^{(i)}, \ F_{\beta}^{(j)} F_{\beta'}^{(j)} = \delta_{\beta\beta'} F_{\beta}^{(j)},$$

$$[E_{\alpha}^{(i)}, F_{\beta}^{(j)}] = 0.$$
(30)

Then, by defining $P(\alpha|i) \stackrel{\text{def}}{=} \langle \Psi | E_{\alpha}^{(i)} | \Psi \rangle$, $P(\beta|j) \stackrel{\text{def}}{=} \langle \Psi | E_{\beta}^{(j)} | \Psi \rangle$, $P(\alpha, \beta|i, j) \stackrel{\text{def}}{=} \langle \Psi | E_{\alpha}^{(i)} E_{\beta}^{(j)} | \Psi \rangle$, a quantum correlation experiment is completely described by the vector

$$(\{P(\alpha|i)\}_{\alpha,i}, \{P(\beta|j)\}_{\beta,j}, \{P(\alpha,\beta|i,j)\}_{\alpha,\beta,i,j}), \tag{31}$$

for $1 \leq \alpha \leq a(i) - 1$, $1 \leq i \leq m$, $1 \leq \beta \leq b(j) - 1$, $1 \leq j \leq n$. The set of these vectors is denoted as $\mathcal{Q}(m,n,a(i),b(j))$. We can easily see that $\mathcal{Q}(m,n,a(i),b(j))$ is isomorphic to $\mathcal{Q}_{\operatorname{Cut}}(m,n)$ when a(i)=b(j)=2 for all i and j. Suppose Υ is the set of all projections I, $E_{\alpha}^{(i)}$ and $F_{\beta}^{(j)}$ for all (α,β,i,j) except (a(i),b(j),i,j); that is, α runs from 1 to a(i)-1 and β runs from 1 to b(j)-1. We represent a product of projections in Υ as a sequence on Υ (e.g. $E_{\alpha}^{(i)}$, $E_{\alpha}^{(i)}$, $E_{\alpha}^{(i)}$, $E_{\alpha}^{(i')}$, $E_{\alpha}^{(i')}$, $E_{\alpha}^{(i')}$, $E_{\alpha}^{(i')}$, are sequences on Υ). For a sequence S, we define the length of S as the minimum number of projections by which we can write S; as a convention, we define the length of I as 0. Then, we define S_c as the set of all sequences whose length is no greater than C; of course, we have $S_c \subseteq S_{c+1}$. Let $S_c = \{S_k\}_{k=1}^{|S_c|}$, where $|S_c|$ is a size of a set S_c . Then, we define a finite set of independent equalities $\mathcal{F}(S_c)$ as a set of equalities of the form

$$\sum_{kl} (F)_{kl} \langle \Psi | S_k S_l | \Psi \rangle = g(P)$$
(32)

which is satisfied by sequences in S_c for an arbitrary choice of projections $\{E_{\alpha}^{(i)}\}_{\alpha=1}^{a(i)}$ and $\{F_{\beta}^{(j)}\}_{\beta=1}^{b(i)}$ satisfying Eq.(30). In Eq.(32), g(P) is an affine function of probabilities $P(\alpha, \beta|i, j)$ defined as

$$g(P) \stackrel{\text{def}}{=} (g)_0 + \sum_{\alpha,\beta,i,j} (g)_{\alpha,\beta,i,j} P(\alpha,\beta|i,j). \tag{33}$$

 $\mathcal{F}(\mathcal{S}_c)$ is not uniquely determined from this definition. But, for all c, there actually exists an easy algorithm to find a set $\mathcal{F}(\mathcal{S}_c)$ satisfying the above condition [20]. Since each equality in $\mathcal{F}(\mathcal{S}_c)$ is determined by a $|\mathcal{S}_c| \times |\mathcal{S}_c|$ matrix F and an affine function k on $\mathbb{R}^{|\mathcal{S}_c|}$, we write $(F, k) \in \mathcal{F}(\mathcal{S}_c)$ if F and k satisfies Eq.(32) in $\mathcal{F}(\mathcal{S}_c)$.

Now, we are ready to present the main result of Navascués et al. [21]. Suppose $Q_c(m, n, a(i), b(j))$ is defined as a set of quantum correlation vectors satisfying the following condition: there exists a $|\mathcal{S}_c| \times |\mathcal{S}_c|$ positive semidefinite matrix $\Gamma \geq 0$ satisfying

$$Tr(F^{T}\Gamma) = g(P) \tag{34}$$

for all $(F,k) \in \mathcal{F}(\mathcal{S}_c)$. We have $\mathcal{Q}_{c+1}(m,n,a(i),b(j)) \subseteq \mathcal{Q}_c(m,n,a(i),b(j))$ Their main result is that

Q(m, n, a(i), b(j)) is actually a limit of the sequence of the sets $\{Q_c(m, n, a(i), b(j))\}_{c=0}^{\infty}$, that is,

$$Q(m, n, a(i), b(j)) = \bigcap_{c=0}^{\infty} Q_c(m, n, a(i), b(j)).$$
(35)

Moreover, by the definition, a quantum correlation vector P is in $\mathcal{Q}_c(m, n, a(i), b(j))$, if and only if

$$\max\{\lambda \mid \Gamma - \lambda I \ge 0,$$

$$\operatorname{Tr}(F^{T}\Gamma) = q(P), \forall (F, k) \in \mathcal{F}(\mathcal{S}_{c})\} > 0.$$

Since the above optimization problem is an SDP, we can check whether P is in $\mathcal{Q}_c(m, n, a(i), b(j))$ by an SDP of the size $|\mathcal{S}_c| \times |\mathcal{S}_c|$. Thus, we can judge whether P is in $\mathcal{Q}_c(m, n, a(i), b(j))$ by

this infinite sequence of SDPs. In [21], they also gave a condition such that if it is satisfied by Γ corresponding to a positive λ , then we can immediately conclude $P \in \mathcal{Q}(m, n, a(i), b(j))$, without having to solve an infinite sequence of SPDs.

Navascués et al.'s method can be applied to the calculation of maximal violation of Bell inequalities. That is, we can always derive an upper bound of the maximal violation by optimizing Bell inequalities over $Q_c(m, n, a(i), b(j))$, and this optimization is also SDP [21]. Suppose we are interested in a Bell inequality $J(P) = \sum_{\alpha,\beta,i,j} V(\alpha,\beta,i,j) P(\alpha,\beta|i,j)$, for some coefficients $V(\alpha,\beta,i,j)$. Then, the optimization of J(P) over $Q_c(m,n,a(i),b(j))$ reduces to the following SDP:

$$\max\{J(P)|P \in \mathcal{Q}_{c}(m, n, a(i), b(j))\}$$

$$= \max\{\operatorname{Tr}(\zeta_{c}\Gamma) \mid \Gamma \geq 0,$$
and $\operatorname{Tr}(F^{T}\Gamma) = g(P), \forall (F, k) \in \mathcal{F}(\mathcal{S}_{c})\}.$ (36)

In the above equation, the $|\mathcal{S}_c| \times |\mathcal{S}_c|$ matrix ζ_c is defined as follows: Since each index of the matrix ζ_c is associated to a sequence in \mathcal{S}_c , we directly represent each index by the corresponding sequence. Then, $(\zeta_c)_{E_{\alpha}^{(i)},F_{\beta}^{(j)}} = V(\alpha,\beta,i,j)/2$ and $(\zeta_c)_{S,S'} = 0$ for all other combination of sequences $(S,S') \in \mathcal{S}_c \times \mathcal{S}_c$. By Eq.(35), we can easily see that Eq.(36) actually converge to the maximal violation of J(P).

Also very recently, Doherty et al. derived a sequence of SDPs which converge to the maximal violation of a Bell inequality [11]. In this final part of this section, we review their result. Suppose \mathcal{P} is a collection of Hermitian polynomials defined as follows: As variables we consider $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$. The number of variables is equal to the number of projections which appear in the quantum correlation experiment, and are labeled in the same way as the projections. We should note that $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$ are non-commutative variables, and do not necessary satisfy condition Eq.(30). We define a set of polynomials $\mathcal{T}_1, \mathcal{T}_2, \mathcal{T}_3, \mathcal{T}_4, \mathcal{T}_5$ on non-commutative variables $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$ as follows:

$$\mathcal{T}_{1} = \left\{ i[E_{\alpha}^{(i)}, F_{\beta}^{(j)}] \middle| 1 \leq \alpha \leq a(i), \\
1 \leq \beta \leq b(j), 1 \leq i \leq m, 1 \leq j \leq n \right\} \\
\mathcal{T}_{2} = \left(\bigcup_{i} \left\{ I - \sum_{\alpha} E_{\alpha}^{(i)} \right\} \right) \cup \left(\bigcup_{j} \left\{ I - \sum_{\beta} F_{\beta}^{(j)} \right\} \right) \\
\mathcal{T}_{3} = \left(\bigcup_{i,\alpha} \left\{ (E_{\alpha}^{(i)})^{2} - E_{\alpha}^{(i)} \right\} \right) \cup \left(\bigcup_{j,\beta} \left\{ (F_{\beta}^{(j)})^{2} - F_{\beta}^{(j)} \right\} \right) \\
\mathcal{T}_{4} = \left\{ i[E_{\alpha}^{(i)}, E_{\alpha'}^{(i)}] \right\}_{\alpha \neq \alpha', i} \cup \left\{ j[F_{\beta}^{(j)}, F_{\beta'}^{(j)}] \right\}_{\beta \neq \beta', j} \\
\mathcal{T}_{5} = \left\{ E_{\alpha}^{(i)} E_{\alpha'}^{(i)} + E_{\alpha'}^{(i)} E_{\alpha}^{(i)} \right\}_{\alpha \neq \alpha', i} \cup \left\{ F_{\beta}^{(j)} F_{\beta'}^{(j)} + F_{\beta'}^{(j)} F_{\beta}^{(j)} \right\}_{\beta \neq \beta', j}. \tag{37}$$

We define $\mathcal{T} = \mathcal{T}_1 \cup \mathcal{T}_2 \cup \mathcal{T}_3 \cup \mathcal{T}_4 \cup \mathcal{T}_5$, and $\mathcal{P} = \mathcal{T} \cup -\mathcal{T}$. Then, for a Hermitian $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$, P is actually a set of Hermitian polynomials. We should note that values of all polynomial in \mathcal{P} are zero for $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$ satisfying Eq.(30). Then, we define the

convex cone $C_{\mathcal{P},c}$ as follows: q is in $C_{\mathcal{P},c}$, then q is a polynomial on $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$ whose order is no greater than 2c, and which has the form $q = \sum_{i} r_{i}^{\dagger} r_{i} + \sum_{i} \sum_{j} s_{ij}^{\dagger} p_{i} s_{ij}$, where $p_{i} \in \mathcal{P}$, and r_{i} , s_{ij} are arbitrary polynomials on $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$. Suppose a polynomial q_{ν} on $\{E_{\alpha}^{(i)}\}_{\alpha,i}$ and $\{F_{\beta}^{(j)}\}_{\beta,j}$ is defined as

$$q_{\nu} = \nu I - \left(\sum_{\alpha,\beta,i,j} V(\alpha,\beta,i,j) E_{\alpha}^{(i)} F_{\beta}^{(j)}\right). \tag{38}$$

Then, the optimization problems

$$w_c \stackrel{\text{def}}{=} \min\{\nu | q_{\nu} \in \mathcal{C}_{\mathcal{P},c}\}$$
 (39)

converge to the maximal violation of the Bell inequality J(P) in the limit $c \to \infty$. Moreover, surprisingly, w_c can also be calculated by SDP [11]. So, this optimization also gives another way to calculate an upper bound of maximal violation of a Bell inequality as close as we like by SDP until the limit of our computational power.

Finally, we note one important fact. Even though Q(m, n, a(i), b(j)) can be characterized by a sequence of SDPs, this does not imply that Q(m, n, a(i), b(j)) can be characterized by a polynomial time algorithm. For example, if the convergence of $Q_c(m, n, a(i), b(j))$ to Q(m, n, a(i), b(j)) is slow, then Eq.(35) does not guarantee the existence of such a polynomial algorithm. Actually, we can see a similar situation in the characterization of entangled states. The set of all separable (non-entangled) states can be characterized by a sequence of SDPs. However, the problem to check whether a given state is separable or not is actually NP-hard [18]. It is an important and interesting open question to see whether or not a similar result holds for quantum correlation vectors.

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A Clifford algebra

In this appendix, we give several important properties of the Clifford algebra associated to a real linear space $V = \mathbb{R}^n$, which are used in this paper. All of the facts given in this appendix can be found in [24, 30].

The Clifford algebra Cl(V) associated to a real linear space $V = \mathbb{R}^n$ is defined to be the quotient algebra $T(V)/\mathcal{I}(V)$, where $T(V) \stackrel{\text{def}}{=} \bigoplus_{r=0}^{\infty} V^{\otimes r}$ is the tensor of V, and $\mathcal{I}(V)$ is the ideal of T(V) generated by all element of the form $v \otimes v - \langle v|v \rangle 1$ for $v \in V$. Although this is the definition of Clifford algebra, the following well-known characterization is more convenient in this paper.

Theorem 4 Let e_1, \dots, e_n be any orthonormal basis of a real linear space V, then, Cl(V) is generated by e_1, \dots, e_n subject to the relations

$$e_i e_j + e_j e_i = 2\delta_{ij}. (40)$$

Thus, a set of all elements in the form $e_{i_1} \cdots e_{i_k}$ with $i_1 < \cdots < i_k$ is a basis of Clifford algebra Cl(V), and the dimension of Cl(V) is 2^n .

In this paper, we are interested in the "complex representation" of Clifford algebra Cl(V), which is a real algebra homomorphism from Cl(V) onto an algebra of all linear operators $\mathfrak{B}(\mathcal{H})$ on a complex finite-dimensional Hilbert space \mathcal{H} . The following property of irreducible complex representations of $Cl(\mathbb{R}^n)$ is important for our paper.

Theorem 5 For even n, up to equivalence of representations, $Cl(\mathbb{R}^n)$ has only one complex irreducible representation, whose dimension is $2^{\frac{n}{2}}$, and which is faithful. For odd n, up to equivalence of representations, $Cl(\mathbb{R}^n)$ has only two different complex irreducible representations, whose dimensions are $2^{\frac{n-1}{2}}$, and which are not faithful.

We can make these irreducible representations in the following way. Suppose $n=2\nu$ is even, and $\mathcal{H}=\mathbb{C}^2$ is a ν -qubit Hilbert space. Then, on \mathcal{H} , the Weyl-Brauer matrices are defined as

$$X_{i} \stackrel{\text{def}}{=} \underbrace{Z \otimes \cdots \otimes Z}_{i-1} \otimes X \otimes \underbrace{I \otimes \cdots \otimes I}_{i-1},$$

$$X_{i+\nu} \stackrel{\text{def}}{=} -\underbrace{Z \otimes \cdots \otimes Z}_{i-1} \otimes Y \otimes \underbrace{I \otimes \cdots \otimes I}_{i-1},$$

$$(41)$$

where X, Y and Z are the Pauli matrices, and an index i satisfies $1 \le i \le \nu$. We can easily check that these matrices satisfy the anti-commutation relation (40). Thus, they are a representation of the generators of $Cl(\mathbb{R}^n)$. Since they also generate the algebra of all linear operators $\mathfrak{B}(\mathcal{H})$ which has the same dimension of $Cl(\mathbb{R}^n)$, this representation is faithful and irreducible. For odd $n = 2\nu + 1$, we can choose an irreducible representation of the generators of the Clifford algebra $Cl(\mathbb{R}^n)$ on a n-qubit Hilbert space \mathcal{H} as $\{X_i\}_{i=1}^{2\nu+1}$

where $\{X_i\}_{i=1}^{2\nu}$ are defined by Eq.(15) and $X_{2\nu+1} \stackrel{\text{def}}{=} \overbrace{Z \otimes \cdots \otimes Z}^{\nu}$. Again, we can check that the anti-commutation relation (40), and $\{X_i\}_{i=1}^{2\nu+1}$ generates the algebra of all linear operators $\mathfrak{B}(\mathcal{H})$, which agrees with the irreducibility of this representation. However, this representation is not faithful, since now the dimension of this algebra is smaller than that of $Cl(\mathbb{R}^n)$. Another inequivalent irreducible representation is derived by redefining $-X_i$ as X_i for $1 \leq i \leq \nu$.

B Review of the binary representation of the stabilizer formalism

In Section 6 of this paper, we use the *binary representation* of the stabilizer formalism. For readers who are not familiar with this topic, we give a small review of it. All the detailed proofs of the statements that appear in the following part can be found in [15] and [28].

First, we rewrite the Pauli matrices by using binary indices as $I = \sigma_{00}, X = \sigma_{01}, Y = \sigma_{11}, Z = \sigma_{10}$. Then, this notation gives an encoding of the Pauli matrices into the binary field \mathbb{Z}_2 as

$$I \leftrightarrow 00, \ X \leftrightarrow 01, \ Y \leftrightarrow 11, \ Z \leftrightarrow 10.$$
 (42)

More generally, we can encode the tensor products of Pauli matrices into a vector space on the binary field as:

$$\sigma_{(\vec{u},\vec{v})} \stackrel{\text{def}}{=} \sigma_{u_1 v_1} \otimes \cdots \otimes \sigma_{u_N v_N}$$

$$\leftrightarrow (u_1 \cdots u_N | v_1 \cdots v_N)^T,$$
(43)

where $\vec{u} \stackrel{\text{def}}{=} (u_1 \cdots u_N)$, $\vec{v} \stackrel{\text{def}}{=} (v_1 \cdots v_N)$, and T is transposition. We can easily see this representation satisfies $\sigma_{(\vec{u},\vec{v})}\dot{\sigma}_{(\vec{u'},\vec{v'})} = \alpha\sigma_{(\vec{u}\oplus\vec{u'},\vec{v}\oplus\vec{v'})}$, where α is a phase factor which ranges over $\{\pm 1, \pm i\}$ depending on $\vec{u}, \vec{v}, \vec{u'}, \vec{v'}$, and \oplus is bitwise summation in the binary field. Since the Pauli group on n-qubits \mathcal{P}_n can be written as

$$\mathcal{P}_n = \{ \alpha \sigma_{(\vec{u}, \vec{v})} | \alpha \in \{\pm 1, \pm i\}, \vec{u}, \vec{v} \in \mathbb{Z}_2^n \}, \tag{44}$$

Eq.(43) gives a representation of the n-qubits Pauli group on the 2n dimensional vector space on binary fields \mathbb{Z}_2^{2n} ; this representation is not faithful since we omit the phase factor α in Eq.(44). We should note that the correspondence (43) can be also understood as giving the projective representation of the finite field \mathbb{Z}_2^{2n} on n-qubits Hilbert space.

Suppose P is a $2n \times 2n$ binary matrix defined as $P \stackrel{\text{def}}{=} \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}$, where I is an $n \times n$

identity matrix. Then, " $\sigma_{(\vec{u},\vec{v})}$ commutes with $\sigma_{(\vec{u'},\vec{v'})}$, if and only if $(\vec{u},\vec{v})P(\vec{u'},\vec{v'})^T=0$." Thus, commutativity of elements of the Pauli group is equivalent to the orthogonality of the corresponding binary vectors under the symplectic inner product; $(\vec{u},\vec{v})P(\vec{u'},\vec{v'})^T$ is called the symplectic inner product between (\vec{u},\vec{v}) and $(\vec{u'},\vec{v'})$. Further, suppose S is a commutative subgroup of the Pauli group on an N qubit system. Then, we can easily see the following fact: $\{X_i\}_{i=1}^m$ are m independent generators of S if and only if a set of vectors $\{\vec{e_k}\}_{k=1}^m$ on \mathbb{Z}_2^{2N} corresponding to $\{X_i\}_{i=1}^m$ is an orthogonal basis of a subspace \mathfrak{S} of \mathbb{Z}_2^{2N} corresponding to S in terms of the symplectic inner product; in other words, the generator matrix $E \stackrel{\text{def}}{=} (\vec{e_1}, \cdots, \vec{e_m})$ satisfies $E^T P E = 0$. In this case, dim $\mathfrak{S} = m$ and all pairs of different vectors \vec{e} and \vec{f} on \mathfrak{S} satisfy $\vec{e}^T P \vec{f} = 0$. In particular, the stabilizer group S of an N-qubit stabilizer state corresponds to an N dimensional self-dual subspace \mathfrak{S} ; that is, \mathfrak{S} is equal to its symplectic orthogonal complement $\mathfrak{S}^c \stackrel{\text{def}}{=} \{\vec{e} \in \mathbb{Z}_2^{2N} | \vec{e}^T P \vec{f} = 0 \ (\forall \vec{f} \in \mathfrak{S})\}$.

Although a stabilizer group of a stabilizer state determines a corresponding self-dual subspace, a given N-dimensional self-dual subspace of a binary field, or a given generator matrix does not uniquely determine a corresponding stabilizer group and a stabilizer state. This fact can be seen as follows: Suppose $\{M_i\}_{i=1}^N$ is a set of commutative and independent Pauli operators on N-qubit Hilbert space, and E is a generator matrix corresponding to $\{M_i\}_{i=1}^N$. Then, for all $(c_1, \dots, c_n) \in \mathbb{Z}_N$, $\{(-1)^{c_i}M_i\}_{i=1}^N$ has the same matrix E as its corresponding generator matrix. In this case, although a stabilizer state $|\Psi\rangle$ corresponding to $\{(-1)^{c_i}M_i\}_{i=1}^N$ is not a stabilizer state corresponding to $\{M_i\}_{i=1}^N$, $|\Psi\rangle$ is a simultaneous eigenvector of $\{M_i\}_{i=1}^N$.

Suppose $\{\vec{e}_k\}_{k=1}^N$ is an orthogonal basis of a self dual subspace \mathfrak{S}_N , and suppose R is an $N \times N$ invertible binary matrix. Then, a set of vectors $\{\vec{f}_l\}_{l=1}^N$ defined by

$$\vec{f_l} \stackrel{\text{def}}{=} \sum_{k=1}^{N} \vec{e_k} R_{kl} \tag{45}$$

is another orthogonal basis of \mathfrak{S}_N . Suppose $\{X_k\}_{k=1}^N$ are independent generators of a stabilizer group S_N , $\{\vec{e_k}\}$ are their binary representation, and R is an $N \times N$ invertible

binary matrix. Then, $\{a_k Y_k\}_{k=1}^N$ is another set of independent generators of S_N , where $a_k \in \{\pm 1, \pm i\}$ is a suitably chosen phase factor, and Y_k is an element of the Pauli group corresponding to a vector $\vec{f_k}$ defined by Eq.(45). Note that if Y_k corresponds to the binary vector $\vec{f_k}$, then, $\pm Y_k$ and $\pm i Y_k$ also correspond to $\vec{f_k}$.

The Clifford group \mathcal{G}_N is defined as the set of all unitary operators satisfying $U\mathcal{P}_N U^{\dagger} \subset \mathcal{P}_N$ for the N qubits Pauli group \mathcal{P}_N . We can easily see that an element U of Clifford group \mathcal{G}_N induces the linear transformation $f_U: \mathbb{Z}_2^{2N} \to \mathbb{Z}_2^{2N}$. In this case, it is known that the set of such transformations $\{f_U\}_{U \in \mathcal{G}_N}$ coincides with the set of all symplectic transformation on \mathbb{Z}_2^{2N} . Thus, for an element of the Clifford group $U, U\sigma_{\vec{e}}U^{\dagger} = a\sigma_{\vec{e'}}$ for a suitably chosen $a \in \{\pm 1, \pm i\}$, if and only if there exists a symplectic matrix Q_U (a matrix satisfying $Q_U^T P Q_U = P$) such that $f_U(\vec{e}) = Q_U \vec{e} = \vec{e'}$.

C Computational investigation of the strength of the nosignalling inequalities

We may wonder to what extent the inclusion (29) is essentially stronger than Tsirelson's construction. In this appendix we review an investigation of a set of known Bell inequalities computationally, showing that in most cases a tighter bound on quantum violation is achieved by using the no-signalling conditions. In some cases, however, the bounds are identical.

Takahashi et al. [25] report on a computational investigation of the optimal value of Bell inequalities with the following constraints:

- (i) the elliptope $\varepsilon(\nabla K_{m,n})$
- (ii) the elliptope $\varepsilon(\nabla K_{m,n})$ and the rooted semimetric polytope $\mathrm{RMet}(\nabla K_{m,n})$

The optimal values were calculated by the method of Avis, Imai and Ito [2] using the software SDPA [14] for a set of 89 Bell inequalities [19], which includes two quantum correlation functions: A2 (the CHSH inequality) and A8 (the I_{3322} inequality [8]), and the other 87 quantum correlation vectors. The results are reproduced here as Table 1. As A2 and A8 are quantum correlation functions, it is consistent with Tsirelson's Theorem 1 that both optimal values are the same. On the other hand, we also see that for two Bell inequalities, A19 and A56, both optimal values coincide. This means that, for the Bell inequalities A19 and A56, the rooted semimetric polytope RMet($\nabla K_{m,n}$) is inactive.

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Table 1: The values of optimum solutions of the semidefinite programming problems for those 89 Bell inequalities [19]

	(i)	(ii)		(i)	(ii)		(i)	(ii)		(i)	(ii)		(i)	(ii)
A 1	0.250	0.000	A19	1.500	1.500	A37	1.550	1.314	A55	1.483	1.380	A73	2.280	2.090
A2	0.414	0.414	A20	1.703	1.560	A38	1.584	1.273	A56	1.717	1.717	A74	2.060	1.830
A3	0.750	0.732	A21	1.250	1.167	A39	1.645	1.399	A57	1.704	1.565	A75	1.981	1.687
A4	0.969	0.817	A22	1.669	1.516	A40	1.676	1.392	A58	1.769	1.564	A76	1.733	1.420
$\mathbf{A5}$	1.245	1.056	A23	1.643	1.283	A41	1.677	1.273	A59	1.833	1.380	A77	2.091	1.776
A6	1.348	1.027	A24	1.685	1.388	A42	1.667	1.431	A60	1.482	1.161	A78	2.193	2.106
A7	1.339	1.078	A25	1.599	1.380	A43	1.672	1.407	A61	1.631	1.205	A79	1.882	1.571
A8	1.183	1.183	A26	1.660	1.280	A44	1.570	1.437	A62	1.528	1.199	A80	1.486	1.220
A9	1.446	1.208	A27	1.618	1.511	A45	1.494	1.322	A63	1.601	1.312	A81	1.908	1.724
A10	1.444	1.106	A28	1.590	1.527	A46	1.570	1.255	A64	1.644	1.229	A82	1.629	1.369
A11	1.442	1.208	A29	1.631	1.298	A47	1.443	1.336	A65	1.598	1.132	A83	2.023	1.764
A12	1.463	1.245	A30	1.730	1.243	A48	1.414	1.294	A66	1.610	1.360	A84	1.972	1.791
A13	1.376	1.143	A31	1.684	1.299	A49	1.605	1.270	A67	1.690	1.258	A85	2.006	1.819
A14	1.471	1.283	A32	1.662	1.161	A50	1.579	1.410	A68	1.647	1.276	A86	2.075	1.850
A15	1.558	1.337	A33	1.624	1.459	A51	1.686	1.565	A69	1.716	1.469	A87	2.037	1.817
A16	1.554	1.252	A34	1.545	1.410	A52	1.665	1.501	A70	1.829	1.612	A88	1.584	1.370
A17	1.486	1.122	A35	1.678	1.403	A53	1.702	1.563	A71	1.757	1.388	A89	2.215	1.420
A18	1.484	1.144	A36	1.662	1.224	A54	1.690	1.489	A72	2.103	1.784			

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