

New Bell inequalities for the singlet state: Going beyond the Grothendieck bound.

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Contemporary versions of Bell's argument against local hidden variable (LHV) theories are based on the Clauser Horne Shimony and Holt (CHSH) inequality, and various attempts to generalize it. The amount of violation of these inequalities cannot exceed the bound set by the Grothendieck constants. However, if we go back to the original derivation by Bell, and use the perfect anti-correlation embodied in the singlet spin state, we can go beyond these bounds. In this paper we derive two-particle Bell inequalities for traceless two-outcome observables, whose violation in the singlet spin state go beyond the Grothendieck constant both for the two and three dimensional cases. Moreover, creating a higher dimensional analog of perfect correlations, and applying a recent result of Alon and his associates (*Invent. Math.* 163 499 (2006)) we prove that there are two-particle Bell inequalities for traceless two-outcome observables whose violation increases to infinity as the dimension and number of measurements grow. Technically these result are possible because perfect correlations (or anti-correlations) allow us to transport the indices of the inequality from the edges of a bipartite graph to those of the complete graph. Finally, it is shown how to apply these results to mixed Werner states, provided that the noise does not exceed 20%.

I. INTRODUCTION

The impossibility of reproducing all correlations observed in composite quantum systems using local hidden variables (LHV) was proven in 1964 by Bell. In his work [1], Bell showed that all local models satisfy the Bell inequalities, but there are measurements on quantum states that violate a Bell inequality. Contemporary versions of the argument are based on the Clauser Horne Shimony Holt (CHSH) inequality [2], rather than the original inequality derived by Bell. There is a very good reason for that. While Bell's argument applied only to the singlet state, the CHSH inequality is violated by all pure entangled states [3], and also by certain mixtures, provided they are not too noisy. From an experimental point of view this is a substantial difference.

However, if we are interested in the question what is the maximal possible violation of any two-particle Bell inequality it is profitable to go back to the original version of Bell (or its simplification by Wigner [4]). Bell is using the perfect

anti-correlation embodied in the singlet spin state. This means that when the spin measurements performed on both sides are along the same direction the outcomes are always opposite. A LHV theory that attempts to reproduce an experiment on the singlet state is thus further constrained.

In this paper I shall show how this can increase the violation in the singlet spin state beyond the Grothendieck constants [5], both for the two and three dimensional cases. Moreover, using the theorem of Tsirelson [6], we can create an analog of perfectly correlated two particle states in any dimension n . Applying a recent result of Alon et.al.[7] I prove that there are Bell inequalities whose violation *increases to infinity* with n . This should be compared with the traditional approach, based on extensions of the CHSH, where the violation cannot increase beyond a finite bound. Technically this outcome is possible because perfect correlations (or anti-correlations) allow us to transport the indices of the inequality from the edges of a bipartite graph to those of the complete graph.

Furthermore, I show how to extend these considerations to mixed Werner states [8], in fact to all mixtures in which the anti correlations are sufficiently close to -1 (or to $+1$). Here we do not get as good results as those obtained by CHSH. However, we show that the new inequalities are robust against quite a bit of noise.

Let Alice and Bob share a singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|+\rangle |-\rangle - |-\rangle |+\rangle) \quad (1)$$

Consider a spin measurement along the \mathbf{x} direction performed by Alice, and along the \mathbf{y} direction by Bob (all Bob's parameters will be denoted with y 's Alice's with x 's). The operator corresponding to both measurement is $S_{\mathbf{x}} \otimes S_{\mathbf{y}}$. The expectation of this operator in the singlet state is $\langle\psi|S_{\mathbf{x}} \otimes S_{\mathbf{y}}|\psi\rangle = -\mathbf{x} \cdot \mathbf{y}$, and in case $\mathbf{x} = \mathbf{y}$ the expectation is -1 . If Alice is choosing her measurements to be in either the \mathbf{x}_1 or \mathbf{x}_2 directions, and Bob is choosing between \mathbf{y}_1 and \mathbf{y}_2 , there are four possible arrangements with the expectations $\langle\psi|S_{\mathbf{x}_i} \otimes S_{\mathbf{y}_j}|\psi\rangle = -\mathbf{x}_i \cdot \mathbf{y}_j$, $i = 1, 2$ and $j = 1, 2$.

A (deterministic) hidden variable theory associates with the physical system a parameter λ whose value determines the outcome of every such experiment. The hidden variable theory is *local* if the value that Alice is measuring does not depend on the direction chosen on Bob's side, and vice versa. Let $X_i(\lambda)$ be the value that Alice is obtaining when the hidden variable has the value λ and the direction on her side is \mathbf{x}_i . By definition $X_i(\lambda) = \pm 1$. Similarly let $Y_j(\lambda)$ be the values measured on Bob's side. Since our LHV is assumed to recover the quantum correlations we expect that when we average the value of $X_i(\lambda)Y_j(\lambda)$ over the space of hidden variables we shall recover the quantum correlations, in other words

$$E(X_i Y_j) \equiv \int X_i(\lambda) Y_j(\lambda) d\mu(\lambda) = \langle\psi|S_{\mathbf{x}_i} \otimes S_{\mathbf{y}_j}|\psi\rangle = -\mathbf{x}_i \cdot \mathbf{y}_j. \quad (2)$$

Here μ is the probability measure on the space of hidden variable. However, LHV theories do not always exist. To see that consider the inequality

$$\frac{1}{2}X_1Y_1 + \frac{1}{2}X_1Y_2 + \frac{1}{2}X_2Y_1 - \frac{1}{2}X_2Y_2 \leq 1, \quad (3)$$

which is satisfied by every choice of values ± 1 to the X_i 's and Y_j 's. This means that the expectations also satisfy

$$\frac{1}{2}E(X_1Y_1) + \frac{1}{2}E(X_1Y_2) + \frac{1}{2}E(X_2Y_1) - \frac{1}{2}E(X_2Y_2) \leq 1. \quad (4)$$

However, if we choose $\mathbf{x}_1 = (-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}, 0)$, $\mathbf{x}_2 = (\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}, 0)$, $\mathbf{y}_1 = (0, -1, 0)$, $\mathbf{y}_2 = (1, 0, 0)$ we have for the quantum expectation values in (2)

$$-\frac{1}{2}\mathbf{x}_1 \cdot \mathbf{y}_1 - \frac{1}{2}\mathbf{x}_1 \cdot \mathbf{y}_2 - \frac{1}{2}\mathbf{x}_2 \cdot \mathbf{y}_1 + \frac{1}{2}\mathbf{x}_2 \cdot \mathbf{y}_2 = \sqrt{2}. \quad (5)$$

This result can be interpreted geometrically as following (see appendix and [9]). In \mathbb{R}^4 consider the convex hull of the 16 vectors of the form $(X_1Y_1, X_1Y_2, X_2Y_1, X_2Y_2)$ where $X_i, Y_j = \pm 1$. This is the *Bell polytope* denoted by $Bell(2, 2)$; all the vectors of the form $(E(X_1Y_1), E(X_1Y_2), E(X_2Y_1), E(X_2Y_2))$ are elements of $Bell(2, 2)$. The inequality (3) is one of its non trivial facets. We normalize this inequality so the constant on the right hand side is 1. In this way the amount of violation of the inequality in (5) indicates how far is the vector $(\mathbf{x}_1 \cdot \mathbf{y}_1, \mathbf{x}_1 \cdot \mathbf{y}_2, \mathbf{x}_2 \cdot \mathbf{y}_1, \mathbf{x}_2 \cdot \mathbf{y}_2) = (-\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})$ lies from the boundary of $Bell(2, 2)$.

It is interesting that we can increase this violation in the case of the singlet. To see that we just repeat, more or less, Bell's original argument [1]. Consider the following inequality which refers only to Alice's hidden variables

$$-X_1X_2 - X_1X_3 - X_2X_3 \leq 1. \quad (6)$$

Assume that the $X_i(\lambda)$, $i = 1, 2, 3$ are the LHV values of the results of Alice's measurements in the direction \mathbf{x}_i . Suppose that Bob chooses his measurements to be in exactly the same directions. If Y_1, Y_2, Y_3 are the hidden variables corresponding to his results then quantum mechanics predicts that $E(X_iY_i) = -\mathbf{x}_i \cdot \mathbf{x}_i = -1$, $i = 1, 2, 3$. Since the X_i, Y_j can have only the values ± 1 we must conclude that $X_i(\lambda) = -Y_i(\lambda)$ for almost all λ (with respect to the probability measure μ on the space of hidden variables), and therefore

$$E(X_iX_j) = -E(X_iY_j) = \mathbf{x}_i \cdot \mathbf{x}_j. \quad (7)$$

From the trivial inequality (6) we have on the other hand: $-E(X_1X_2) - E(X_1X_3) - E(X_2X_3) \leq 1$. However, if we take $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ to be in the same plane and 120° apart we get from (7)

$$-\mathbf{x}_1 \cdot \mathbf{x}_2 - \mathbf{x}_1 \cdot \mathbf{x}_3 - \mathbf{x}_2 \cdot \mathbf{x}_3 = \frac{3}{2} > \sqrt{2}. \quad (8)$$

Here too we can associate a geometric picture with inequality (6). In \mathbb{R}^3 consider the set of 8 vectors of the form (X_1X_2, X_1X_3, X_2X_3) with $X_i = \pm 1$, their convex hull is a polytope $Bell(3)$ and (6) is a facet. Again, we choose the constant on the right hand side of (6) to be 1, and (8) indicates how far is the vector $(\mathbf{x}_1 \cdot \mathbf{x}_2, \mathbf{x}_1 \cdot \mathbf{x}_3, \mathbf{x}_2 \cdot \mathbf{x}_3) = (-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$ from the boundary of $Bell(3)$. More on these polytopes and their generalizations in the appendix.

Note that so far we dealt only with directions \mathbf{x}_i which lie in a two dimensional plane. In the next section we shall see how to use the same method to get a violation in three dimensions above the known upper bounds. This is achieved by the application of a new Bell inequality. More generally, consider the possible extensions of the CHSH method. Define the number $K_G(n)$ - called the Grothendieck constant of order n - to be the least positive real number such that the inequality

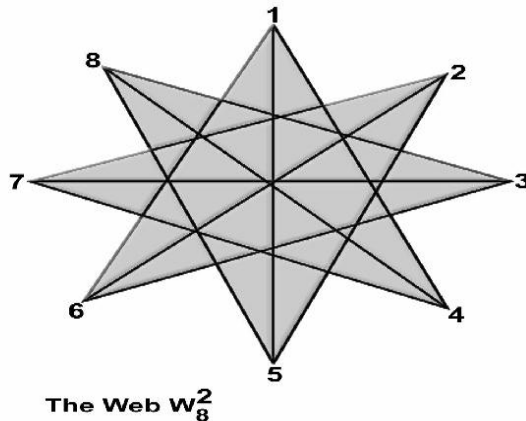
$$\left| \sum_{i=1}^m \sum_{j=1}^m a_{ij} \mathbf{x}_i \cdot \mathbf{y}_j \right| \leq K_G(n) \sup_{X_i, Y_j = \pm 1} \left| \sum_{i=1}^m \sum_{j=1}^m a_{ij} X_i Y_j \right|, \quad (9)$$

is satisfied for every natural number m , every choice of real numbers a_{ij} , $1 \leq i \leq m$, $1 \leq j \leq m$, and every choice of unit vectors $\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{y}_1, \dots, \mathbf{y}_m \in \mathbb{R}^n$. Grothendieck [10] introduced these constants and proved that $K_G = \lim_{n \rightarrow \infty} K_G(n)$ is finite. Tsirelson [6] made the connection with Bell inequalities. It is known that $K_G(2) = \sqrt{2}$, so (5) is the best possible result when all the directions are in the same plane. It is not known whether this is also the best result when we let the directions $\mathbf{x}_i, \mathbf{y}_j$ vary in the three dimensional space. In this case the known bounds are $\sqrt{2} \leq K_G(3) \leq 1.5163$. It is also known that the limit K_G satisfies $1.6770 \leq K_G \leq \pi/(2 \log(1 + \sqrt{2})) = 1.7822$, see [5] for details. Although the last lower bound is better than $\sqrt{2}$, it is very hard to come up with a concrete inequality which will do better than CHSH for any pure quantum state. Finding new Bell inequalities, let alone all of them, is in general computationally hard problem [9]. More on that in the appendix.

However, we have already seen how we can get above $\sqrt{2}$ when we are using perfect correlations. In the next section we shall see that our method leads to a violation above the upper bound for $K_G(3)$ in the three dimensional case. The reason why all this is possible is the following: In the CHSH case (2) the sum is taken over the edges of the bipartite graph $K_{2,2}$, and in the higher dimensional case in equation (9) over $K_{m,m}$. However, in inequality (6) the sum is taken over the edges of the complete graph on 3 vertices K_3 , and this makes the difference. Indeed, let $A(n)$ be the least real number such that

$$\left| \sum_{1 \leq i < j \leq n} a_{ij} \mathbf{x}_i \cdot \mathbf{x}_j \right| \leq A(n) \sup_{X_i = \pm 1} \left| \sum_{1 \leq i < j \leq n} a_{ij} X_i X_j \right| \quad (10)$$

for every choice of reals a_{ij} , $1 \leq i < j \leq n$, and every $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^n$. Then as n grows $A(n)$ becomes unbounded; in a recent paper Alon and his associates [7] extended Grothendieck's work to the complete graph and proved that



$A(n) = \Omega(\log n)$. In section 3 I will note how this theorem is relevant to quantum mechanics.

Finally in section 4 I show how to extend the method to cases where the correlations are not perfect, for example in some mixed Werner states. Although the inequalities are provably robust against quite a bit of noise, the method so far did not lead to results as good as CHSH. Some open questions regarding this point are indicated.

II. THE CLICK-WEB INEQUALITY: GOING ABOVE $K_G(3)$.

Definition 1 Let p, q , and, r be three integers such that $q \geq 2$ and $p - q = 2r + 1$. The web W_p^r is the graph whose set of vertices is $V_p = \{1, 2, \dots, p\}$ and set of edges is $\{i, i + r + 1\}, \dots, \{i, i + r + q\}$; $i = 1, 2, \dots, p$, addition is mod p .

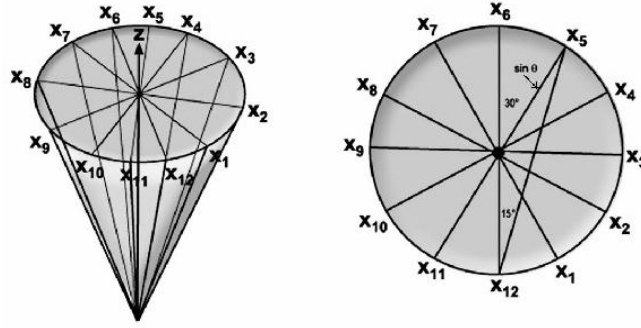
Fig 1 shows the web W_8^2 , the similarity with the spider web is the source of the name.

Alon [11] identified the maximal cuts in W_p^r . Following his result Deza and Laurent were able to find new facets of the cut polytope [12]. The facet inequalities of the cut polytope are very closely related to Bell inequalities (see [12], more on that in the appendix). From their result it is easy to derive the following:

Theorem 1 Let p, q , and, r be three integers such that $q \geq 2$ and $p - q = 2r + 1$. Then the following inequality is satisfied for all $X_1, \dots, X_p, Z_1, \dots, Z_q \in \{-1, 1\}$

$$\sum_{i=1}^p \sum_{j=1}^q X_i Z_j - \sum_{\{i,j\} \in W_p^r} X_i X_j - \sum_{1 \leq i < j \leq q} Z_i Z_j \leq q(r+1). \quad (11)$$

The inequality involves $p + q$ variables X_i and Z_j . They can be taken as the random variables in a LHV theory, representing the outcomes of Alice's spin measurements along the $p + q$ directions \mathbf{x}_i and \mathbf{z}_j in \mathbb{R}^3 . Assuming, as



$$\mathbf{z}=\mathbf{z}_1=\mathbf{z}_2=\mathbf{z}_3$$

The 12-bouquet $p=12, q=3, r=4$

before, that Bob is measuring the spin along the same directions as Alice, and taking the perfect anti-correlation in the singlet state into account, we obtain a contradiction with the LHV model when

$$V_p^r = \frac{1}{q(r+1)} \left[\sum_{i=1}^p \sum_{j=1}^q \mathbf{x}_i \cdot \mathbf{z}_j - \sum_{\{i,j\} \in W_p^r} \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{1 \leq i < j \leq q} \mathbf{z}_i \cdot \mathbf{z}_j \right] > 1. \quad (12)$$

Let $p = 12$ and $q = 3, r = 4$, and let $\mathbf{z}_1 = \mathbf{z}_2 = \mathbf{z}_3 = (0, 0, 1)$. For $0 < \theta < \frac{\pi}{2}$ let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{12}$ all satisfy $\mathbf{x}_i \cdot \mathbf{z}_j = \cos \theta$, and be evenly spaced on the circle $\{\mathbf{x} : \mathbf{x} \cdot \mathbf{z}_j = \cos \theta\}$. The vectors $\mathbf{x}_i, \mathbf{z}_j$ look like a bouquet of flowers (figure 2). We have $\mathbf{x}_i \cdot \mathbf{z}_j = \cos \theta, \mathbf{z}_i \cdot \mathbf{z}_j = 1, \mathbf{x}_i \cdot \mathbf{x}_{i+6} = \cos 2\theta, \mathbf{x}_i \cdot \mathbf{x}_{i+5} = \mathbf{x}_i \cdot \mathbf{x}_{i+7} = (1 - 2 \cos^2 \frac{\pi}{12} \sin^2 \theta)$, where the sum in the indices is taken mod 12.

Substituting these values into (12) we get

$$V_{12}^4(\theta) = \frac{36 \cos \theta - 6 \cos 2\theta - 12(1 - 2 \cos^2 \frac{\pi}{12} \sin^2 \theta) - 3}{15}, \quad (13)$$

and $V_{12}^4(\theta) > 1$ for a large range of θ . In particular, $f(0.32477\pi) = 1.5209$ is larger than the upper bound for $K_G(3)$.

Using the same argument with $p = 11, q = 2$, and $r = 4$ we obtain an arrangement called the 11-bouquet with

$$V_{11}^4(\theta) = \frac{22 \cos \theta - 11(1 - 2 \cos^2 \frac{\pi}{22} \sin^2 \theta) - 1}{10}, \quad (14)$$

and $V_{11}^4(0.3303\pi) = 1.5168$.

In this way we can get sequences of independent inequalities, with unbounded number of measurements, all violated by the singlet state. One way to see that is to generalize the above example: we take $p = 2k + 1, q = 2$, and $r = k - 1$, and define the $2k + 1$ -bouquet by taking $\mathbf{z}_1 = \mathbf{z}_2 = (0, 0, 1)$, and $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{2k+1}$ be equally spaced and satisfy

$\mathbf{x}_i \cdot \mathbf{z}_j = \cos \theta$, then

$$V_{2k+1}^k(\theta) = \frac{(2k+1)[2\cos\theta - (1 - 2\cos^2\frac{\pi}{4k+2}\sin^2\theta)] - 1}{2k}, \quad (15)$$

$\lim_{k \rightarrow \infty} V_{2k+1}^k(\theta) = 2\cos\theta - \cos 2\theta$ with the maximum 1.5 obtained at $\theta = \frac{\pi}{3}$.

Another way to obtain infinitely many violated inequalities is to take, for some natural number m , $p = 4m + 1$, $q = 2m$, and $r = m$. Define $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_q$ to be all in the same plane and equally spaced (so they are the roots of unity of order q), similarly let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_p$ be the p roots of unity (the \mathbf{x} 's and \mathbf{z} 's need not be in the same plane). Then $\sum \mathbf{z}_j = 0$ and $\sum_{1 \leq i < j \leq q} \mathbf{z}_i \cdot \mathbf{z}_j = -\frac{q}{2}$, substituting into (12) we obtain a violation when $V_{4m+1}^m > 1$ where

$$V_{4m+1}^m = \frac{1}{2m(m+1)} \left[(4m+1) \sum_{j=1}^m \cos\left(\frac{(2j-1)\pi}{4m+1}\right) + m \right], \quad (16)$$

and indeed $\lim_{m \rightarrow \infty} V_{4m+1}^m = \frac{4}{\pi} = 1.27324$.

III. AN APPLICATION OF TSIRELSON'S THEOREM

We can generalize the above argument using the following result [6],

Theorem 2 *The following conditions on an $n \times n$ matrix (r_{ij}) are equivalent:*

- a. There exists a finite dimensional Hilbert space \mathcal{H} , Hermitian operators $A_1, A_2, \dots, A_n, B_1, B_2, \dots, B_n$, and a state W on $\mathcal{H} \otimes \mathcal{H}$ such that $\text{spectrum}[A_i] \subset [-1, 1]$, $\text{spectrum}[B_j] \subset [-1, 1]$ and $r_{ij} = \text{tr}[W(A_i \otimes B_j)]$ for $i, j = 1, 2, \dots, n$.*
- b. The same as in 1, but with the additional conditions: $A_i^2 = I, B_j^2 = I, \text{tr}[W(A_i \otimes I)] = 0, \text{tr}[W(I \otimes B_j)] = 0, A_{i_1}A_{i_2} + A_{i_2}A_{i_1}$ is proportional to I for all $i_1, i_2 = 1, 2, \dots, n, B_{j_1}B_{j_2} + B_{j_2}B_{j_1}$ is proportional to I for all $j_1, j_2 = 1, 2, \dots, n$, and $\dim \mathcal{H} \leq 2^{\lfloor \frac{n+1}{2} \rfloor}$.*
- c. There exist unit vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ and $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$ in the $2n$ -dimensional real space \mathbb{R}^{2n} such that $r_{ij} = \mathbf{x}_i \cdot \mathbf{y}_j$.*

From which we obtain

Corollary 3 *Given unit vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n \in \mathbb{R}^n$ there is a finite dimensional Hilbert space \mathcal{H} , traceless Hermitian operators $A_1, A_2, \dots, A_n, B_1, B_2, \dots, B_n$ on \mathcal{H} with $\text{spectrum} \pm 1$, a state W on $\mathcal{H} \otimes \mathcal{H}$ such that $\text{tr}[W(A_i \otimes I)] = 0, \text{tr}[W(I \otimes B_j)] = 0, \text{tr}[W(A_i \otimes B_j)] = \mathbf{x}_i \cdot \mathbf{x}_j$. In particular $\text{tr}[W(A_i \otimes B_i)] = 1$.*

To see that just extend the \mathbf{x}_i 's to be $2n$ - dimensional unit vectors by adding zero coordinates, then define $\mathbf{y}_j = \mathbf{x}_j$ and apply Tsirelson's theorem. To make sure that the A_i and B_j are traceless we can always extend the Hilbert space

\mathcal{H} by adding finitely many extra dimensions (without changing the support of W) and making sure that $\text{tr}[A_i] = \text{tr}[B_j] = 0$ by adding ± 1 to their spectrum.

Now, consider a sequence of measurements where Alice and Bob are sharing many copies of the state W , Alice is measuring each one of the operators A_1, A_2, \dots, A_n several times, and Bob the operators B_1, B_2, \dots, B_n . The possible outcomes on each side are ± 1 . A LHV model for this experiment consists of an association of a random variable $X_i(\lambda)$ with every operator A_i , and a random variable $Y_j(\lambda)$ with B_j , such that $X_i(\lambda), Y_j(\lambda) \in \{-1, 1\}$ for every value of the hidden variable λ . To recover the quantum correlation we require that $E(X_i Y_j) = \text{tr}[W(A_i \otimes B_j)] = \mathbf{x}_i \cdot \mathbf{x}_j$. Since we have $E(X_i Y_i) = 1$ we conclude that $X_i(\lambda) = Y_i(\lambda)$ for almost all λ and all $1 \leq i \leq n$. This means that for the purpose of this LHV model W behaves very much like the singlet, only that now the \mathbf{x}_i 's are directions in \mathbb{R}^n .

Charikar and Wirth [13] proved that there is a universal constant $C > 0$ such that

$$\left| \sum_{1 \leq i < j \leq n} a_{ij} \mathbf{x}_i \cdot \mathbf{x}_j \right| \leq C \log n \sup_{X_i = \pm 1} \left| \sum_{1 \leq i < j \leq n} a_{ij} X_i X_j \right| \quad (17)$$

for every real numbers a_{ij} , $1 \leq i < j \leq n$ and all unit vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n \in \mathbb{R}^n$. More important for our purpose, it was lately proved [7] that *this is the best bound*. In other words *there is a universal constant $c > 0$ such that for each n there are real numbers b_{ij} , $1 \leq i < j \leq n$ and unit vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n \in \mathbb{R}^n$ with*

$$\left| \sum_{1 \leq i < j \leq n} b_{ij} \mathbf{x}_i \cdot \mathbf{x}_j \right| > c \log n \sup_{X_i = \pm 1} \left| \sum_{1 \leq i < j \leq n} b_{ij} X_i X_j \right|. \quad (18)$$

Now choose the directions \mathbf{x}_i that are guaranteed by this result and the corresponding quantum system in corrolary 3. Inequality (18) then means that the results of Alice and Bob's measurements $\text{tr}[W(A_i \otimes B_j)] = \mathbf{x}_i \cdot \mathbf{x}_j$ violate local realism by an amount which is unbounded, and increases to infinity with the dimension and with the number of measurements. As noted, this is possible because our LHV theory is constrained to satisfy the condition of perfect correlations. Below we shall see how this condition can be somewhat relaxed.

IV. THE CASE OF WERNER STATES

Let $|\psi\rangle$ be the singlet in (1) and consider the mixed state introduced by Werner [8]

$$\rho_\eta = \eta |\psi\rangle\langle\psi| + \frac{1-\eta}{4} I. \quad (19)$$

here $0 < \eta < 1$ and I the unit operator on the four dimensional complex Hilbert space. If $\eta < \frac{1}{3}$ the state ρ_η is separable and if $\eta > \frac{1}{\sqrt{2}}$ it violates the CHSH inequality (2). The interesting feature of this state is that there are values of η for which ρ_η - although not separable- still admits LHV models of various kinds (for details see [5]). My

purpose here is to show how Bell's original argument can be extended to this case of imperfect correlations. This does not improve the $\frac{1}{\sqrt{2}}$ bound given by CHSH, but better inequalities may do just that.

We have $\text{tr}[\rho_\eta(S_{\mathbf{x}} \otimes S_{\mathbf{y}})] = -\eta \mathbf{x} \cdot \mathbf{y}$, and in particular $\text{tr}[\rho_\eta(S_{\mathbf{x}} \otimes S_{\mathbf{x}})] = -\eta$. As before, let Alice measure the spin in three directions $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ and let Bob measure the spin in the same directions. Assume that $X_i(\lambda) = \pm 1$ is the value assigned to Alice's measurements in the \mathbf{x}_i direction by a LHV model, and likewise let $Y_i(\lambda)$ be Bob's value.

$$E(X_i Y_j) = -\eta \mathbf{x}_i \cdot \mathbf{x}_j, \quad E(X_i Y_i) = -\eta \quad (20)$$

As before, let μ be the probability measure on the space of hidden variables. Put $A_+^j = \{\lambda ; X_j(\lambda) = Y_j(\lambda)\}$ and $A_-^j = \{\lambda ; X_j(\lambda) = -Y_j(\lambda)\}$. Then $\mu(A_+^j) + \mu(A_-^j) = 1$, and by (20): $\mu(A_+^j) - \mu(A_-^j) = -\eta$, hence $\mu(A_+^j) = \frac{1}{2}(1 - \eta)$. Now, let $i \neq j$ then

$$E(X_i X_j) = \int_{A_+^j} X_i Y_j d\mu(\lambda) - \int_{A_-^j} X_i Y_j d\mu(\lambda) = 2 \int_{A_+^j} X_i Y_j d\mu(\lambda) - E(X_i Y_j),$$

and therefore

$$-(1 - \eta) - E(X_i Y_j) \leq E(X_i X_j) \leq (1 - \eta) - E(X_i Y_j). \quad (21)$$

Consider the inequality (6), only written in a slightly different way

$$-X_1 X_2 + X_1 Y_3 + X_2 Y_3 \leq 1. \quad (22)$$

Using (20), and assuming the worst case in (21) we know that the following inequality must be satisfied by the LHV model

$$E(X_1 Y_2) - (1 - \eta) + E(X_1 Y_3) + E(X_2 Y_3) \leq 1 \quad (23)$$

and a violation occurs when $-\eta \mathbf{x}_1 \cdot \mathbf{x}_2 - (1 - \eta) - \eta \mathbf{x}_1 \cdot \mathbf{x}_3 - \eta \mathbf{x}_2 \cdot \mathbf{x}_3 > 1$. If we take the \mathbf{x}_i to be in the same plane and $\frac{2\pi}{3}$ apart we get $\eta > 0.8$.

We can apply the same argument to the clique-web inequality (11) assuming that the X_i 's correspond to measurements made by Alice and the Z_j 's by Bob (which means reversing the directions of the \mathbf{z}_j). Taking into account that $p - q = 2r + 1$ and $|W_p^r| = \frac{pq}{2}$ we get

$$\eta > \frac{p}{(r+1)V_p^r + p - r - 1} \quad (24)$$

where V_p^r is given in (12). If we take the $(2k+1)$ -bouquet in (15) and the limit $k \rightarrow \infty$ we get again $\eta > 0.8$. It is quite possible that a better result can be obtained by choosing other arrangements of unit vectors.

We can apply the same consideration to the state W guaranteed in corollary 3 to Tsirelson's theorem. Define

$$\rho_\eta^W = \eta W + \frac{1-\eta}{d^2} I, \quad (25)$$

where $d = \dim \mathcal{H}$ in corollary 3. Since $\text{tr}[\rho_\eta^W (A_i \otimes B_j)] = \eta \mathbf{x}_i \cdot \mathbf{x}_j$ and in particular $\text{tr}[\rho_\eta^W (A_i \otimes B_i)] = \eta$ we can repeat the same argument. Suppose that b_{ij} satisfy (18), and we normalize it so that $\sup_{X_i = \pm 1} \left| \sum_{1 \leq i < j \leq n} b_{ij} X_i X_j \right| = 1$. In order to minimize the noise we shall choose a subset $J \subset \{1, 2, \dots, n\}$ and associate the random variables $\{X_i ; i \in J\}$ with Alice, and $\{Y_j ; j \in \bar{J}\}$ with Bob. In other words, on the right hand side of 18 we substitute

$$\sum_{1 \leq i < j \leq n} b_{ij} X_i X_j \rightarrow \sum_{i < j, ij \in J} b_{ij} X_i X_j + \sum_{i \in J} \sum_{j \in \bar{J}} b_{ij} X_i Y_j + \sum_{i < j, ij \in \bar{J}} b_{ij} Y_i Y_j.$$

Let $i < j$, if $(i, j) \in (J \times \bar{J}) \cup (\bar{J} \times J)$ then we substitute on the left hand side of (18) $b_{ij} \mathbf{x}_i \cdot \mathbf{x}_j \rightarrow \eta b_{ij} \mathbf{x}_i \cdot \mathbf{x}_j$. If $(i, j) \in (J \times J) \cup (\bar{J} \times \bar{J})$ then we assume worst case and substitute in (18) $b_{ij} \mathbf{x}_i \cdot \mathbf{x}_j \rightarrow \eta b_{ij} \mathbf{x}_i \cdot \mathbf{x}_j - |b_{ij}| (1 - \eta)$. The accumulated noise will be minimized when we choose J for which

$$N\{b_{ij}\} = \min_J \left(\sum_{i < j, ij \in J} |b_{ij}| + \sum_{i < j, ij \in \bar{J}} |b_{ij}| \right) = \min_{Z_j = \pm 1} \frac{1}{2} \sum_{i \neq j} |b_{ij}| (1 + Z_i Z_j), \quad (26)$$

obtains. (That is, we have to solve MAX CUT for the complete graph K_n with weights $|b_{ij}|$, and then subtract the outcome from the total weight $\sum |b_{ij}|$). The condition for LHV model will be violated when

$$\eta > \frac{N\{b_{ij}\} + 1}{N\{b_{ij}\} + \left| \sum_{1 \leq i < j \leq n} b_{ij} \mathbf{x}_i \cdot \mathbf{x}_j \right|}. \quad (27)$$

It is interesting to see whether this expression is bounded from below by a positive constant as $n \rightarrow \infty$, and what the bound is. In fact there are two competing "forces" acting here: In order that (18) be valid $N\{b_{ij}\}$ should be substantial. To take an extreme example, if $N\{b_{ij}\} = 0$ then we are in the bipartite case and the Grothendieck bound holds, so (18) cannot be valid. On the other hand, if $N\{b_{ij}\}$ is too big it can mask the advantage of having $\left| \sum_{1 \leq i < j \leq n} b_{ij} \mathbf{x}_i \cdot \mathbf{x}_j \right|$ in the denominator of (27).

V. APPENDIX

A. Polytopes and complexity

Let $\mathbf{X} = (X_1, X_2, \dots, X_n)$, $\mathbf{Y} = (Y_1, Y_2, \dots, Y_m)$ be vectors with entries in $\{-1, 1\}$. Denote by $\sigma_{ij}(\mathbf{X}, \mathbf{Y}) = X_i Y_j$ and consider it as a vector in \mathbb{R}^{nm} with lexicographic order on the indices. The convex hull, in \mathbb{R}^{nm} , of $\{\sigma_{ij}(\mathbf{X}, \mathbf{Y}); \mathbf{X} \in \{-1, 1\}^n, \mathbf{Y} \in \{-1, 1\}^m\}$ is a polytope, call it $BELL(n, m)$. The face inequalities for $BELL(n, m)$ have the form

$\sum_{i,j} \alpha_{ij} X_i Y_j \leq \alpha$, where α_{ij} and α are real numbers. The inequality is valid if and only if it is satisfied by all the vertices $\sigma_{ij}(\mathbf{X}, \mathbf{Y}) = X_i Y_j$ of $BELL(n, m)$. It represents a *facet* if, in addition, equality holds for a subset of the σ_{ij} 's which spans an affine subspace of co-dimension one. For example the CHSH inequalities (3) are facet inequalities of $BELL(2, 2)$, and all the non-trivial inequalities of that polytope have that same shape.

A related structure is the polytope $BELL(n)$: Given $\mathbf{X} = (X_1, X_2, \dots, X_n) \in \{-1, 1\}^n$ define $\sigma_{ij}(\mathbf{X}) = X_i X_j$ for $1 \leq i < j \leq n$ and consider $\sigma_{ij}(\mathbf{X})$ as a vector in $\mathbb{R}^{\frac{1}{2}n(n-1)}$. $BELL(n)$ is the convex hull of $\{\sigma_{ij}(\mathbf{X}); \mathbf{X} \in \{-1, 1\}^n\}$ in $\mathbb{R}^{\frac{1}{2}n(n-1)}$. For both $BELL(n, m)$ and $BELL(n)$ finding all the inequalities is an impossible task (see below). In this paper we are using the fact that more inequalities are known for $BELL(n)$ than for the general case $BELL(n, m)$. Since the singlet state entails $X_i = -Y_i$ when Alice and Bob are measuring in the same directions, we can use the known inequalities of $BELL(n)$. Note also the following relation between the polytopes: Let $u \in BELL(n)$ be a $\frac{1}{2}n(n-1)$ -dimensional vector, define $v \in \mathbb{R}^{n^2}$ by $v_{ij} = v_{ji} = u_{ij}$ when $1 \leq i < j \leq n$ and $v_{ii} = 1$, then $v \in BELL(n, n)$. This means that every valid inequality for $BELL(n, n)$ can be collapsed to a valid inequality for $BELL(n)$. Moreover, if deciding membership in $BELL(n)$ is a computationally hard task, then so is deciding membership in $BELL(n, n)$.

Similarly, Let $\mathbf{a} = (a_1, a_2, \dots, a_n) \in \{0, 1\}^n$ for $1 \leq i < j \leq n$ denote $\delta_{ij}(\mathbf{a}) = a_i \oplus a_j = a_i + a_j - 2a_i a_j$ and consider it as a vector in $\mathbb{R}^{\frac{1}{2}n(n-1)}$. The cut polytope $CUT(n)$ is the convex hull of $\{\delta_{ij}(\mathbf{a}); \mathbf{a} \in \{0, 1\}^n\}$. The relations between $CUT(n)$ and $BELL(n)$ are not hard to determine. Since for all $1 \leq i < j \leq n$

$$\delta_{ij}(\mathbf{a}) = a_i \oplus a_j = \frac{1 - X_i X_j}{2} = \frac{1 - \sigma_{ij}(\mathbf{X})}{2} \quad \text{where } X_i = 2a_i - 1 \quad (28)$$

we conclude that $(v_{ij}) \in BELL(n)$ if and only if $(\frac{1}{2}(1 - v_{ij})) \in CUT(n)$. There is extensive work on the facets of the cut polytope [12]. Each facet inequality can be readily transferred to $BELL(n)$.

Finally, let $\mathbf{b} = (b_1, b_2, \dots, b_n) \in \{0, 1\}^n$, for $1 \leq i \leq j \leq n$ denote $\pi_{ij}(\mathbf{b}) = b_i b_j$ and consider it as a vector in $\mathbb{R}^{\frac{1}{2}n(n+1)}$ with lexicographic order on the indices. The convex hull in $\mathbb{R}^{\frac{1}{2}n(n+1)}$ of $\{\pi_{ij}(\mathbf{b}); \mathbf{b} \in \{0, 1\}^n\}$ is called correlation polytope, and denoted by $COR(n)$. (Note that $COR(n)$ has dimension $\frac{1}{2}n(n+1)$ while $CUT(n)$ and $BELL(n)$ have dimension $\frac{1}{2}n(n-1)$). For these polytope we have: [12, 14]

Theorem 4 (a) Let $(p_{ij}) \in \mathbb{R}^{\frac{1}{2}n(n+1)}$ then $(p_{ij}) \in COR(n)$ if and only if there is a probability space (X, Σ, μ) and events $E_1, E_2, \dots, E_n \in \Sigma$ such that $p_{ij} = \mu(E_i E_j)$ for $1 \leq i \leq j \leq n$. (b) Let $(c_{ij}) \in \mathbb{R}^{\frac{1}{2}n(n-1)}$ then $(c_{ij}) \in CUT(n)$ if and only if there is a probability space (X, Σ, μ) and events $E_1, E_2, \dots, E_n \in \Sigma$ such that $c_{ij} = \mu(E_i \triangle E_j) = \mu[(E_i \setminus E_j) \cup (E_j \setminus E_i)] = \mu(E_i) + \mu(E_j) - 2\mu(E_i E_j)$ for $1 \leq i < j \leq n$.

For both the cut polytope and the correlation polytope we can easily extend the definition to the bipartite cases

$CUT(n, m)$ and $COR(n, m)$ in a straightforward way. The relations between the one-sided polytopes and their bipartite versions are similar to that of the Bell polytope..

For the correlation polytope we have the following complexity results [10] which can easily be transferred to the cut polytope and the Bell polytope.

1. Deciding whether a given rational $(p_{ij}) \in \mathbb{R}^{\frac{1}{2}n(n+1)}$ is an element of $COR(n)$ is an NP -complete problem .
(This remains valid when $p_{ii} = \frac{1}{2}$ for all $1 \leq i \leq n$.)
2. Deciding whether a given inequality is *not* valid for $COR(n)$ is an NP -complete problem.

All this means that unless $NP = P$ (or at least $NP = coNP$) deriving all the inequalities for any of these polytopes is a computationally impossible task for large n . This does not prevent us from deriving special cases or even infinite families of inequalities.

B. The Clique-Web inequalities of $CUT(n)$

A graph $G = (V, E)$ consists of a set of vertices $V_n = \{1, 2, \dots, n\}$ and a set of edges E , which are just pairs of vertices. We shall always assume that if $\{i, j\} \in E$ then $i \neq j$. (Note, we do *not* assume directionality, so that $\{i, j\} = \{j, i\}$ is the same edge). If the set of vertices V_n has been fixed we shall often speak loosely on ‘the graph E ’ mentioning only the edges. The set of all pairs on n vertices is called the *complete* graph and denoted by K_n .

Let $S \subset V_n = \{1, 2, \dots, n\}$ be a non empty subset of vertices. Denote by $\kappa(S) = \{\{i, j\}; i \neq j, i, j \in S\}$. If $\kappa(S) \subset E$ then $\kappa(S)$ is called a clique in the graph $G = (V_n, E)$. Also, define a graph $\delta(S) = \{\{i, j\}; i \in S, j \notin S \text{ or } i \notin S, j \in S\}$. The graph $\delta(S)$ is called *a cut* (or a cut in K_n). Denote by $\mathbf{a} = (a_1, a_2, \dots, a_n) \in \{0, 1\}^n$ the indicator function of S , so that $a_i = 1$ for $i \in S$ and $a_i = 0$ otherwise. Then $\{i, j\} \in \delta(S)$ if and only if $a_i \oplus a_j = a_i + a_j - 2a_i a_j = 1$. Hence, the vertices of the cut polytope $CUT(n)$, that is $\delta_{ij}(\mathbf{x}) = a_i \oplus a_j$, are the indicator functions of the cuts $\delta(S)$.

The inequalities that we have considered follow from a precise characterization of $\delta(S) \cap E$ for a graph related to W_p^r . Recall that if p, q , and, r ne three integers such that $q \geq 2$ and $p - q = 2r + 1$ the *web* W_p^r is the graph whose set of vertices is $V_p = \{1, 2, \dots, p\}$ and set of edges is $\{i, i + r + 1\}, \dots, \{i, i + r + q\}; i = 1, 2, \dots, p$, addition is mod p . The *antiweb* AW_p^r is the complement in K_p of the web W_p^r .

For these graphs Alon [11] proved the following

Theorem 5 *Let p, r be integers such that $p \geq 2r + 3, r \geq 1$. Let $S \subset \{1, 2, \dots, p\}$ and assume that $|S| = s$.*

1. *If $s \leq r$, then $|\delta S \cap AW_p^r| \geq s(2r + 1 - s)$, with equality if and only if $\kappa(S)$ is a clique in AW_p^r .*

2. If $r + 1 \leq s \leq \frac{p}{2}$, then $|\delta S \cap AW_p^r| \geq r(r + 1)$ with equality if and only if S is an interval in $\{1, 2, \dots, p\}$, that is, it has the form $S = \{i, i + 1, i + 2, \dots, i + s - 1\}$ for some i , $1 \leq i \leq p$ (addition is mod p .)

As an outcome of Alon's theorem Deza and Laurent proved the following inequality for $CUT(p + q)$ where ($q = p - 2r - 1$):

$$\sum_{\{i,j\} \in W_p^r} a_i \oplus a_j + \sum_{1 \leq i < j \leq q} b_i \oplus b_j - \sum_{i=1}^p \sum_{j=1}^q a_i \oplus b_j \leq 0 \quad (29)$$

(See [12] for details). Here $\mathbf{a} = (a_1, a_2, \dots, a_p) \in \{0, 1\}^p$ and $\mathbf{b} = (b_1, b_2, \dots, b_q) \in \{0, 1\}^q$. If we substitute $X_i = 2a_i - 1$ and $Z_j = 2b_j - 1$ and use the identity (28), we get the inequality (11) for $BELL(p + q)$.

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