Maximal Violation of the Collins-Gisin-Linden-Massar-Popescu Inequality for Infinite Dimensional States

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We present a much simplified version of the Collins-Gisin-Linden-Massar-Popescu inequality for the $2 \times 2 \times d$ Bell scenario. Numerical maximization of the violation of this inequality over all states and measurements suggests that the optimal state is far from maximally entangled, while the best measurements are the same as conjectured best measurements for the maximally entangled state. For very large values of d the inequality seems to reach its minimal value given by the probability constraints. This gives numerical evidence for a tight quantum Bell inequality (or generalized Csirelson inequality) for the $2 \times 2 \times \infty$ scenario.

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The violation of Bell inequalities [1] by certain quantum correlations can be seen as a nonclassical property of those correlations. This "quantum nonclassicality" has its roots in quantum entanglement. There are several ways to quantify entanglement of which one is the so-called entanglement entropy of a quantum state [2]. Quantum states with maximal entanglement entropy, so-called maximally entangled states, play an important role in quantum information science [3]. It was long believed that the maximally entangled state must also be the "most nonclassical" state in the sense of maximal violation of Bell inequalities. Although this is true for the CHSH inequality [4], it was given evidence in [5,6] that this is not true for the more complex Collins-Gisin-Linden-Massar-Popescu (CGLMP) inequality [7], as also exposed in [8].

In the following, we investigate maximal nonclassicality in the context of the CGLMP. We present a new simplified version of the CGLMP inequality. As in [5,6] numerical analysis suggests that the optimal state for each number of outcomes above $d = 2$ is not maximally entangled, where we mainly work with the assumption that the dimension of the Hilbert space D is equal to the number of outcomes d as in [5,6], but also investigate the case of $d < D$ and the validity of this assumption. We give numerical evidence that the best measurements are the well-known (conjectured) best measurements with the maximally entangled state. The simple form of our new version of CGLMP enables us to effectively extend the numerical search to a number of measurement outcomes and dimension of the Hilbert spaces of the order of 10^6. We observe that for these large values of d the new version of CGLMP seems to reach its absolute bound at the boundary of the polytope of all probability vectors. This gives numerical evidence for the tightness of a quantum Bell inequality (or generalized Csirelson inequality) for the $2 \times 2 \times \infty$ scenario.

The $2 \times 2 \times d$ Bell scenario and a new version of the CGLMP inequality.—Let us consider the standard scenario of the CGLMP inequality [7] which consists of two spacelike separated parties, Alice and Bob. Both share a copy of a pure state $|\psi\rangle \in \mathbb{C}^D \otimes \mathbb{C}^D$ on the composite system. Let Alice and Bob have a choice of performing two different projective measurements which each can have d possible outcomes, where $d \leq D$. We call this a $2 \times 2 \times d$ scenario.

Let A_a^i, $a = 1, 2$ and $i = 0, \ldots, d - 1$ denote the positive operators corresponding to Alice's measurement a with outcome i and similar for Bob, B_b^j. They satisfy $\sum_{i=0}^{d-1} A_a^i = \mathbb{1}$. The probability predicted by quantum mechanics (QM) that Alice obtains the outcome i and that Bob obtains the outcome j conditioned on Alice has chosen measurement a and Bob measurement b then reads

$$\mathbb{P}_Q(i, j|a, b) = \mathrm{Tr}(A_a^i \otimes B_b^j |\psi\rangle\langle\psi|). \quad (1)$$

Let us on the other hand consider the framework of local realistic (LR) theories, where the joint probability distribution can be written as

$$\mathbb{P}_L(i, j|a, b) = \sum_\lambda p(\lambda)\mathbb{P}(i|a, \lambda)\mathbb{P}(j|b, \lambda), \quad (2)$$

meaning that conditioned on their mutual past the probability distributions of Alice and Bob are uncorrelated.

As already mentioned, QM is nonclassical in the sense that there exist joint probability distributions $\mathbb{P}_Q(i, j|a, b)$ arising from QM which do not admit a local realistic representation in the form of (2). Bell [1] was the first to put this statement into a testable form in terms of an inequality which is violated for nonclassical probability distributions.

We now give a new Bell inequality for the $2 \times 2 \times d$ Bell scenario:

$$\mathbb{P}_L(A_2 < B_2) + \mathbb{P}_L(B_2 < A_1) + \mathbb{P}_L(A_1 < B_1) + \mathbb{P}_L(B_1 \leq A_2) \geqslant 1, \quad (3)$$

where $\mathbb{P}_L(A_a < B_b) = \sum_{i<j} \mathbb{P}_L(i, j|a, b)$.

This inequality can be easily proven. Let us start with the following obvious statement: $\{A_2 \geq B_2\} \cap \{B_2 \geq A_1\} \cap \{A_1 \geq B_1\} \subseteq \{A_2 \geq B_1\}$. Taking the complement we get $\{A_2 < B_1\} \subseteq \{A_2 < B_2\} \cup \{B_2 < A_1\} \cup \{A_1 < B_1\}$. This implies for the probabilities that $\mathbb{P}_L(A_2 < B_1) = 1 - \mathbb{P}_L(A_2 \geq B_1) \leq \mathbb{P}_L(A_2 < B_2) + \mathbb{P}_L(B_2 < A_1) + \mathbb{P}_L(A_1 < B_1)$, which completes the proof.

The new version (3) of the CGLMP inequality has apart from its simple form several advantages over previous versions. One advantage is that the inequality does not depend on the actual values of the measurement outcomes, only their relative order on the real line matters. For the case of measurements with outcomes $0, \ldots, d-1$ this inequality implies another simplified version of the CGLMP inequality presented in [5], as well as the original CGLMP inequality. Another advantage is that inequality (3) reads the same for all values of d. Further, the way the new inequality is derived might be interesting for finding new, simpler inequalities for other Bell settings, such as the $2 \times 3 \times 2$ Bell setting.

In the following section we will investigate the maximal violation of inequality (3) by QM for large values of the number of outcomes and dimension of the Hilbert space.

Violation of the CGLMP inequality for the maximally entangled state—In the following we will assume that the dimension of the Hilbert space D is equal to the number of outcomes d which we abbreviate as dimension d. We will comment on this assumption at the end of this Letter, where we also present numerical evidence for the validity of this assumption. For the maximally entangled state, $|\Phi\rangle = \sum_{i=0}^{d-1} |ii\rangle/\sqrt{d}$, it has long been conjectured that the measurements which maximally violate the CGLMP inequality are described by operators A_a and B_b with the following eigenvectors [7,9]:

$$|i\rangle_{A,a} = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} \exp\left(\mathbf{i}\frac{2\pi}{d}k(i+\alpha_a)\right)|k\rangle_A, \tag{4}$$

$$|j\rangle_{B,b} = \frac{1}{\sqrt{d}} \sum_{l=0}^{d-1} \exp\left(\mathbf{i}\frac{2\pi}{d}l(-j+\beta_b)\right)|l\rangle_B, \tag{5}$$

where the phases read $\alpha_1 = 0$, $\alpha_2 = 1/2$, $\beta_1 = 1/4$, and $\beta_2 = -1/4$, here $\mathbf{i} = \sqrt{-1}$ is the imaginary number.

We evaluate the left-hand side of inequality (3) for the joint probabilities arising from QM in the case of the maximally entangled state and the just described measurements. For later purposes we will leave the Schmidt coefficients unspecified throughout this calculation and only equate them to $1/\sqrt{d}$ at the end. We use (1), where the $A_a^i = |i\rangle_{A,a}\langle i|_{A,a}$ are the projectors on the corresponding eigenspaces defined in (4) and (5) and similarly for B_b^j. We obtain

$$\mathcal{A}_d(\psi) \equiv \mathbb{P}_Q(A_2 < B_2) + \mathbb{P}_Q(B_2 < A_1) + \mathbb{P}_Q(A_1 < B_1) + \mathbb{P}_Q(B_1 \leq A_2) = \sum_{i=0}^{d-1}\sum_{j=0}^{d-1} M_{ij}\lambda_i\lambda_j, \tag{6}$$

where the $d \times d$ matrix M can be simplified to

$$M_{ij} = 2\delta_{ij} - \frac{1}{d}\cos^{-1}\left(\frac{(i-j)\pi}{2d}\right). \tag{7}$$

Putting $\lambda_i = 1/\sqrt{d}$, i.e., looking at the maximally entangled state, we obtain for $d = 2$, $\mathcal{A}_2(\Phi) = (3-\sqrt{2})/2 \approx 0.792\,89$ which corresponds to the maximal violation of the CHSH inequality know from Csirelson's inequality [10].

It is also interesting to look at the conjectured (it is not known that these are the best measurements) maximal violation of (3) with the infinite dimensional maximally entangled state. We get $\lim_{d\to\infty}\mathcal{A}_d(\Phi) = 2 - 16\,\mathrm{Cat}^2/\pi^2 \approx 0.515$ where Cat is Catalan's constant, reproducing the result obtained in [7] for the original version of the CGLMP inequality.

In this section we described what are believed to be the best measurements for the CGLMP inequality with the maximally entangled state. Though it is often thought that the maximally entangled state $|\Phi\rangle$ represents the most nonclassical quantum state, evidence has been given in [5,6] that the states which maximally violate inequality (3) are not maximally entangled. In the following section we provide further evidence for this and investigate several properties of the optimal state especially in the case of very large values of d.

On the maximal violation of the CGLMP inequality—In the previous section we described the measurements which in the case of the maximally entangled state appear to give the maximal violation of inequality (3). However, as mentioned above, it has already been given evidence that in the case of $d \geq 3$ the state that causes the maximum violation of the inequality is actually not the maximally entangled state [5,6].

In the following we want to optimize the left-hand side of inequality (3) over all possible measurements and states. For this purpose we assume that the state of Alice's and Bob's composite system is a pure state $|\psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$ and that the measurements A_a and B_b describing Alice's and Bob's measurement are projective and nondegenerate as also considered above.

For small values of d we can numerically perform the optimization. The results for the first values are summarized in Table I. Shown are the minimal values of the left-hand side of inequality (3), denoted by $\min\mathcal{A}_d(\psi, A_a, B_b)$, and the Schmidt coefficients of the optimal state for which $\mathcal{A}_d(\psi, A_a, B_b)$ reaches its minimum.

One observes that for $d \geq 3$ the optimal state is not maximally entangled. More precisely, as we will see later the entanglement entropy decreases as d becomes bigger.

TABLE I. Violation of the CGLMP inequality.

d	$\min\mathcal{A}$	λ_0	λ_1	λ_2	λ_3	λ_4
2	0.7929	0.7071	0.7071	⋯	⋯	⋯
3	0.6950	0.6169	0.4888	0.6169	⋯	⋯
4	0.6352	0.5686	0.4204	0.4204	0.5686	⋯
5	0.5937	0.5368	0.3859	0.3859	0.3859	0.5368

The optimal states arising from the numerical optimization over $\mathcal{A}_d(\psi, A_a, B_b)$ agree with results obtained in [6], but differ from the results in [5]. That is because in [5] the quantity to be optimized was not the CGLMP inequality, but the Kullback-Leibler divergence (relative entropy) which contrary to common belief is not equivalent to the concept of maximal violation of Bell inequalities [12].

Closer analysis of the optimal measurements A_a^i and B_b^j shows that even though the optimal state is not the maximally entangled state the best measurements seem to be the best measurements (4) and (5) of the previous case. Further numerical optimizations for higher values of d give strong evidence that this is true in general.

If we assume that (4) and (5) are the best measurements for all values of d we can further simplify the optimization. We have already derived in Eq. (6) that in the case of the measurements (4) and (5) we can write $\mathcal{A}_d(\psi) = \sum_{i=0}^{d-1}\sum_{j=0}^{d-1} M_{ij}\lambda_i\lambda_j$, where $|\psi\rangle = \sum_{i=0}^{d-1}\lambda_i|ii\rangle$ and the $d \times d$ matrix M was given in (7).

Hence under this assumption, finding the maximal violation of (3) reduces to finding the smallest eigenvalue of the matrix M. The corresponding eigenvector $\{\lambda_i\}_{i=0}^{d-1}$ gives us the optimal state.

For $d = 2, 3$ we obtain $\min\mathcal{A}_2 = (3 - \sqrt{2})/2$, with $\vec{\lambda} = (1, 1)^T/\sqrt{2}$, and $\min\mathcal{A}_3 = (12 - \sqrt{33})/9$, with $\vec{\lambda} = (1, \gamma, 1)^T/(\sqrt{2 + \gamma^2})$, and $\gamma = (\sqrt{11} - \sqrt{3})/2$, agreeing with results presented in [6] where violations of the original CGLMP inequality were investigated.

More interesting becomes the search for eigenvectors with minimal eigenvalue for a large number of possible measurement outcomes. Numerical search for those eigensystems is feasible for very large values of d by use of Arnoldi iteration.

The results of the numerical optimizations are summarized in Fig. 1. Shown is the minimal target value $\mathcal{A}_d(\psi)$ as a function of the dimension d for a range from 2 to 10^6 both for the case of the maximally entangled state and the optimal state. In the case of the maximally entangled state, $\mathcal{A}_d(\Phi)$ approaches very quickly the asymptotic value $\mathcal{A}_\infty(\Phi) \approx 0.515$ derived above.

In the case of the optimal state it is interesting that the maximal violation of (3) does not approach an asymptote very quickly. In fact, for very large d it falls off slower than logarithmically with the dimension. The numerical data shown in Fig. 1 do suggest that the minimal value of $\mathcal{A}_d(\psi)$ approaches zero as d tends to infinity. This is very interesting since zero is the absolute minimum of $\mathcal{A}_d(\psi)$ on the boundary of the polytope of all probability vectors. If one could show analytically that there exists an optimal state which actually causes $\mathcal{A}_d(\psi)$ to approach zero as d tends to infinity, one would have proven a new tight quantum Bell inequality for the $2 \times 2 \times \infty$ scenario (see conjecture at the end of this section).

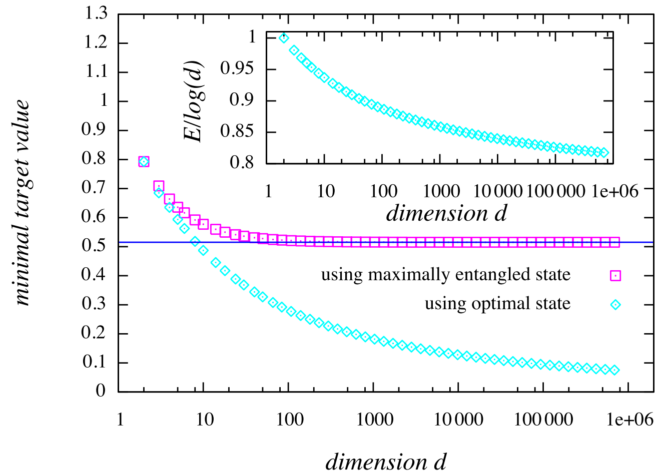

FIG. 1 (color online). Minimal value of the left-hand side of inequality (3) as a function of the dimension d: (i) for the maximally entangled state and (ii) for the optimal state. Inside: Entanglement entropy $E/\log d$ of the optimal state as a function of the dimension d.

Let us now investigate further properties of the optimal states causing the maximal violation of inequality (3). Figure 2 shows the typical shape of a optimal state for $d \geq 3$, namely, in the case of $d = 10\,000$. Plotted are the Schmidt coefficients λ_i as a function of the index i. The reflection symmetry around $(d-1)/2$ can be easily derived from the specific form of the symmetric kernel M_{ij}.

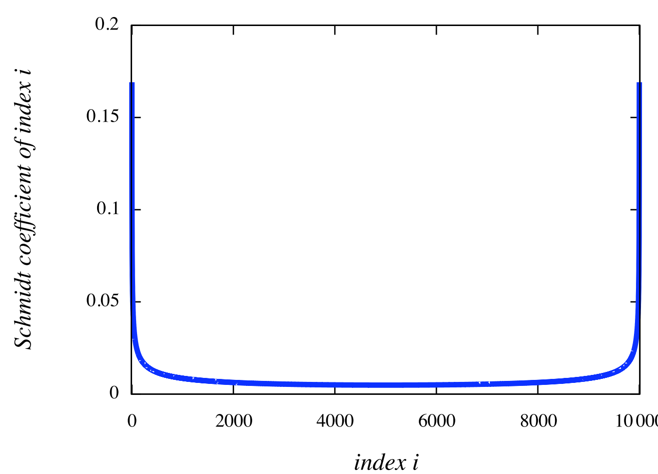

FIG. 2 (color online). The typical shape of a optimal state for $d \geq 3$. Shown are the Schmidt coefficients λ_i of the optimal state for $d = 10\,000$ as a function of the index i.

As d increases the Schmidt coefficient get more and more peaked at $i = 0$ and $i = d - 1$.

It is also interesting to look at the entanglement entropy of the optimal state. Whereas for the maximally entangled state $E(\Phi)/\log d = 1$ for all values of d, in the case of the optimal state the entanglement entropy decreases with the dimension. As in the case of the minimal value of $\mathcal{A}_d(\psi)$ the entanglement entropy decreases slower than logarithmically, but we are not able to give an asymptotic bound for it. This is contrary to work presented in [5], where the entanglement entropy seemed to approach the asymptotic value $\lim_{d\to\infty} E(\psi) = \ln d \approx 0.69 \log d$. Again, the disagreement is due to the fact that in the latter the quantity to be optimized was not the CGLMP inequality, but rather the Kullback-Leibler divergence.

From the insights gained in this section we state the following conjecture:

Conjecture (Quantum Bell inequality): For $d \to \infty$ the minimal value of $\mathbb{P}_Q(A_2 < B_2) + \mathbb{P}_Q(B_2 < A_1) + \mathbb{P}_Q(A_1 < B_1) + \mathbb{P}_Q(B_1 \leq A_2)$ converges to zero, where the best measurements for each d are the ones presented above, (4) and (5), and the optimal states are of the form shown in Fig. 2. Hence,

$$\begin{aligned} \mathbb{P}_Q(A_2 < B_2) + \mathbb{P}_Q(B_2 < A_1) + \mathbb{P}_Q(A_1 < B_1) \\ + \mathbb{P}_Q(B_1 \leq A_2) \geqslant 0 \end{aligned} \tag{8}$$

is a *tight* quantum Bell inequality for the $2 \times 2 \times \infty$ Bell setting.

The fact that the inequality seems to reach its minimal value given by the probability constraints as $d \to \infty$ also relates to recent results derived in [13] for a chained version of the CGLMP inequality.

Conclusion.—A new version of the CGLMP inequality for the $2 \times 2 \times d$ Bell scenario has been presented. Numerically, under the assumption that the number of outcomes is equal to the dimension of the Hilbert space D, the optimal states are not maximally entangled for $d \geq 3$, though the best measurements with respect to those states are the same as for the maximally entangled state.

We investigated the maximal violation of this new inequality for very large numbers of measurement outcomes and dimension of the Hilbert space. We analyzed the specific form of the best states and their entanglement entropy. It turned out that for increasing dimension the entanglement entropy of the optimal state decreases, agreeing with the observations made in [5,6]. Interestingly, the numerics indicate that the maximal violation of the inequality tends, as the number of measurement outcomes and dimension of the Hilbert space tends to infinity, to the absolute bound imposed by the polytope of probability vectors. We conjectured from this a tight quantum Bell inequality for the $2 \times 2 \times \infty$ Bell scenario. An analytical proof of the tightness of this inequality is work in progress which will hopefully appear soon.

To justify the above assumption that the dimension of the Hilbert space D is equal to the number of possible outcomes d we also numerically analyzed the case of $d < D$. In particular, we obtained the minimal target value optimized over Schmidt coefficients and all possible combinations of degenerate measurements A_1, A_2, B_1, B_2 for $d = 2, 3, 4$ with $D = 5$ and over randomly selected degenerate measurements for $d = 2, 3, 4, 5$ with $D = 20$. In all cases the smallest obtained target values agreed with the corresponding minimal target values obtained under the assumption that $D = d$ as summarized in Table I up to an error of 10^{-3}. This gives strong evidence for the validity of the assumption that $D = d$ and suggests that the minimal target values obtained under this assumption are also valid for the case of degenerate projective measurements and POVM measurements which can always be realized as projective measurements on a higher-dimensional Hilbert space due to Naimark's theorem. Further, it strengthens the evidence that the optimal state for $d > 2$ is not maximally entangled beyond the analysis of [5,6].

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