Maximal violation of the I3322 inequality using infinite dimensional quantum systems

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The I3322 inequality is the simplest bipartite two-outcome Bell inequality beyond the Clauser-Horne-Shimony-Holt (CHSH) inequality, consisting of three two-outcome measurements per party. In case of the CHSH inequality the maximal quantum violation can already be attained with local two-dimensional quantum systems, however, there is no such evidence for the I3322 inequality. In this paper a family of measurement operators and states is given which enables us to attain the largest possible quantum value in an infinite dimensional Hilbert space. Further, it is conjectured that our construction is optimal in the sense that measuring finite dimensional quantum systems is not enough to achieve the true quantum maximum. We also describe an efficient iterative algorithm for computing quantum maximum of an arbitrary two-outcome Bell inequality in any given Hilbert space dimension. This algorithm played a key role to obtain our results for the I3322 inequality, and we also applied it to improve on our previous results concerning the maximum quantum violation of several bipartite two-outcome Bell inequalities with up to five settings per party.

I. INTRODUCTION

One of the most puzzling features of quantum theory is its nonlocal nature. Separated observers on a shared entangled state may carry out measurements on such a way that the correlations they generate are outside the set of common cause correlations [1]. In particular, such quantum correlations may find application in novel device-independent information tasks, which have no counterparts in the classical world. They enable perfect security [2], randomness generation [3] and state tomography [4] without the need to trust the internal working of the devices.

The concept of Bell inequalities is a particularly useful tool to detect nonlocal quantum correlations, as violation of a single Bell inequality conclusively proves the nonlocal character of correlations. The standard scenario for a bipartite two-outcome Bell test is as follows. Two spacelike separated parties, Alice and Bob, both share copies of a quantum state $|\psi\rangle$ of a given dimension $n \times n$. Alice (Bob) may choose between $m_A$ ($m_B$) alternative measurements at random, where each measurement has two possible outcomes $\{0,1\}$. In a single run of the experiment the correlations between the two $\{0,1\}$-valued observables $A_i$ and $B_j$ can be represented by the product $A_iB_j$. In order to obtain an accurate estimation of the correlations for each pair $(i,j)$, Alice and Bob repeat the experiment many times using a copy of the state $|\psi\rangle$ in each round. Averaging over many runs of the experiment yields the mean value $\langle A_iB_j \rangle$.

The CHSH inequality [5] is probably the most well-known and simplest example of a Bell inequality consist-

\[ \langle A_1B_1 \rangle + \langle A_1B_2 \rangle + \langle A_2B_1 \rangle - \langle A_2B_2 \rangle - \langle A_1 \rangle - \langle B_1 \rangle \leq 0. \]

Curiously, quantum theory allows for a violation of the CHSH inequality, but the strength of nonlocal correlations is still limited, it obeys

\[ \langle A_1B_1 \rangle + \langle A_1B_2 \rangle + \langle A_2B_1 \rangle - \langle A_2B_2 \rangle - \langle A_1 \rangle - \langle B_1 \rangle \leq 1/\sqrt{2} - 1/2. \]

where now the expectation values can be expressed by $\langle A_iB_j \rangle = \langle \psi|A_i \otimes B_j|\psi\rangle$, $\langle A_i \rangle = \langle \psi|A_i \otimes I_B|\psi\rangle$, $\langle B_j \rangle = \langle \psi|I_A \otimes B_j|\psi\rangle$, $i,j = 1,2$ with $\{0,1\}$-valued observables $A_i$, $B_j$. According to Tsirelson’s theorem [6], the bound applies to any quantum correlations without making assumptions on the sort of measurements or the dimensionality of the states involved. Though, the maximum value of $1/\sqrt{2} - 1/2$ can already be achieved with a maximally entangled two-qubit state.

Inequalities, whose bound are saturated with quantum correlations without relying on dimensionality such as in Eq. (2) were coined as quantum Bell inequalities [7]. There exist various methods in the literature [8-10], to cite just a few, which enable one to derive quantum Bell inequalities. Also, several explicit constructions exist in the literature (e.g., [11-14]), including so-called irrelevant ones [15] (where the classical and quantum limits coincide). The method invented by Navascués, Pironio and Acín (NPA) [11] is based on the solution of a hierarchy of semidefinite programming (SDP) relaxations and is particularly useful since it gives better and better upper bounds on the maximum violation of an arbitrary Bell inequality by stepping to higher levels in the hierarchy. Moreover, the series of upper bounds in the hierarchy

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keep to the exact quantum maximum in terms of commuting measurements \[11,16\]. On the other hand, one can use heuristic algorithms to obtain nontrivial lower bounds in some finite dimensional Hilbert spaces on Bell inequalities, recovering the explicit form of the states and measurement operators as well. If the above computed upper and lower bounds coincide within numerical accuracy for a given Bell inequality, then we may say that a quantum Bell inequality has been obtained, which delimits the boundary of the quantum domain.

In particular, in our previous papers \[13,17\] we computed lower bounds on the maximum quantum violations and determined the corresponding measurement operators and state vectors with two different methods, both involved some parametrization of the operators and applying a downhill simplex method to find the optimum parameters. The disadvantage of these methods is that the size of the Hilbert space was very limited. We could actually handle systems of maximum eight dimensional real or six dimensional complex component spaces. Different sizes of component spaces require different parametrizations for the operators, hence in order to extend these methods to a higher dimension would involve working out an appropriate parametrization. Moreover, the choice of measurement operators were also limited. For example, in the case of eight dimensional component spaces only projection operators projecting onto four dimensional subspaces were allowed.

In spite of the limitations we could get the maximum quantum violation of the great majority of inequalities we considered (the list comprises 241 bipartite Bell inequalities with up to five settings per party collected from Refs. \[13,18,19\] and detailed results concerning their optimum violations are presented in the web page \[20\]). However, there were still a few exceptions, where the upper bound value resulting from the NPA method \[10\] did not match the best lower bound result. The most interesting one was the case of \(I_{3322}\). This is the smallest case we considered, and perhaps the simplest tight Bell inequality after the CHSH one, with only three measurement settings per party. It was introduced by Froissart \[21\] back in 1981, and recently reinvented in Refs. \[22,23\]. It reads

\[
I_{3322} = \langle A_2 \rangle - \langle B_1 \rangle - 2 \langle B_2 \rangle + \langle A_1 B_1 \rangle + \langle A_1 B_2 \rangle + \langle A_2 B_1 \rangle + \langle A_2 B_2 \rangle - \langle A_1 B_3 \rangle - \langle A_2 B_3 \rangle - \langle A_3 B_1 \rangle + \langle A_3 B_2 \rangle \leq 0. \tag{3}
\]

In a local classical model we have the maximum value of 0, while the largest violation one could get with qubits was 0.25, which could already be achieved with a maximally entangled pair of qubits (see e.g., \[11,13,16\]). On the other hand, the best upper bounds are based on the NPA method \[10\] and at level three it yields the significantly higher upper bound, 0.250 875 56 \[11,16\]. We could even go above level three to an intermediate level in \[13\], and presently we have got the upper bound 0.250 875 38 at level four. From the dependence of the bound on the level it was derived it seemed to be clear that it would not go much lower (note also that the computational complexity of the SDP problem increases dramatically with higher levels of relaxations). In fact, it is the above observation, which motivated us to search for a quantum violation beyond the two-qubit value of 0.25.

In the present paper we set out to resolve the puzzling problem concerning the maximum quantum violation of the \(I_{3322}\) inequality. To this end, we introduce in Sec. \[11\] an efficient iterative algorithm which was applied to explore the largest quantum violation of \(I_{3322}\) for states up to local dimension 20. Sec. \[11\] contains the main results, presenting the explicit construction of states and measurement operators, which give by means of an iterative method the conjectured maximal quantum value of \(I_{3322}\) in function of the dimensionality. In particular, for dimensions very large we recover the upper bound computed with the NPA method at level four within high numerical accuracy, thereby establishing a quantum Bell inequality for \(I_{3322}\). We note that the optimal quantum state in the infinite dimensional space is far from the maximally entangled state, thereby supporting the claim that entanglement and nonlocality are different resources \[24\]. In Sec. \[11\] we investigate the remaining 19 Bell inequalities from a set of 241 inequalities (plus two additional symmetric 4-setting inequalities from Ref. \[23\]), where the tightness of the quantum bound could not be proven previously, and in some of the remaining cases now we manage to close the gap. Sec. \[11\] summarizes the results achieved.

II. THE ITERATIVE ALGORITHM

As mentioned above, the drawback of our previous heuristic methods in Refs. \[13,17\] for computing lower bounds on the maximum quantum violation of Bell inequalities is that the size of the local Hilbert space we could handle is limited up to dimension eight. With the iterative method we introduce here for two-outcome Bell inequalities we can go to higher dimensions, which is only limited by the computational difficulties due to the increasing complexity of the problem with increasing Hilbert space dimensions. Similarly to the previous methods, this algorithm does not guarantee to converge to the global optimum solution. In case of larger spaces we may miss it even after tens of thousands of restarts with different initial values. Nevertheless, it managed to find every optima we derived with our previous methods, and in almost all cases it has done it considerably faster.

The problem to be solved consists of maximizing the quantum value of the Bell expression with coefficients \(M_{\mu \nu}\), which can be written as:

\[
Q = \max \sum_{\mu=0}^{m_\mu} \sum_{\nu=0}^{m_\nu} M_{\mu \nu} \langle \psi | \hat{A}_\mu \otimes \hat{B}_\nu | \psi \rangle, \tag{4}
\]
where there are $m_A$ and $m_B$ measurement settings for Alice and Bob, respectively, $\hat{A}_\mu$ ($1 \leq \mu \leq m_A$) and $\hat{B}_\nu$ ($1 \leq \nu \leq m_B$) are the measurement operators of Alice and Bob, respectively, $\hat{I}_A = \hat{I}_A$ and $\hat{I}_B = \hat{I}_B$ are unit operators in the component spaces, and $|\psi\rangle$ is the state vector. The maximum can always be reached by a pure state. In case of two-outcome measurements it is enough to consider projection operators as the measurement operators \cite{12}. When there are only two parties, a further simplification is that when we take a matrix representation of the expression above, we may choose the bases in the component spaces such that they correspond to the Schmidt decomposition of the state vector $|\psi\rangle$. If we confine ourselves to $n$-dimensional component spaces we get:

$$ Q_n = \max_{\mu=0}^{m_A} \sum_{\nu=0}^{m_B} \sum_{i=1}^{n} \sum_{j=1}^{n} M_{\mu\nu} A_{ij}^\mu B_{ij}^\nu \lambda_i \lambda_j, $$

where $A_{ij}^\mu$ and $B_{ij}^\nu$ are components of matrices of $\hat{A}_\mu$ and $\hat{B}_\nu$, respectively, and $\lambda_i$ are the Schmidt coefficients of the state vector. If $n$ is smaller than the dimensionality of the component spaces required for the maximum quantum violation, then $Q_n \leq Q$.

To solve the problem first we choose appropriate random matrices and numbers for Bob’s measurement operators, and for $\lambda_i$. To get the matrices, first we take a diagonal matrix with zero and one diagonal values chosen randomly, then we apply many random two dimensional unitary (or if we confine ourselves to real matrices, orthogonal) transformations. For $\lambda_i$ we take positive numbers between zero and one from a uniform distribution, then we normalize them. In the iterative algorithm the first step is to calculate the optimal measurement operators of Alice, given Bob’s operators and the state vector. This can be done directly. Equation (5) can be rewritten as:

$$ Q_n = \max_{\mu=0}^{m_A} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}^\mu X_{ji}^\mu = \max_{\mu=0}^{m_A} \sum_{i=0}^{m_A} \text{Tr}(\hat{A}_\mu \hat{X}_\mu), $$

where

$$ X_{ji}^\mu = \sum_{\nu=0}^{m_B} M_{\mu\nu} B_{ij}^\nu \lambda_i \lambda_j, $$

We can get the matrix of the optimum $\hat{A}_\mu$ ($1 \leq \mu \leq m_A$) the following way. First we diagonalize the matrix of $\hat{X}_\mu$. Then we create a diagonal matrix. We choose its diagonal matrix element one where the diagonalized matrix of $\hat{X}_\mu$ contains a positive number, and zero otherwise. Then we transform this matrix with the inverse of the transformation that diagonalized the matrix of $\hat{X}_\mu$. To show that this is the matrix of the optimal $\hat{A}_\mu$ we note that trace is invariant to basis transformation, and it is easy to see that the optimum matrix of projector $\hat{A}_\mu$ in the basis diagonalizing $\hat{X}_\mu$ is the one we have chosen.

The second step is to derive Bob’s optimal matrices while Alice’s matrices and the state vector are fixed. This can be done equivalently to the first step. These two steps are the same as the steps of the see-saw algorithm by Werner and Wolf \cite{29}, who used it to get maximum violation with fixed (not necessarily pure) states. A variant of the see-saw algorithm for Bell inequalities with multiple outcomes was also devised \cite{27, 28}.

In the third step the best state vector is calculated for the measurement operators. It is done the same way as in our previous method \cite{13}. An algorithm applying this very third step has been also used by Liang et al. \cite{29} to compute quantum optima for multiple-outcome Bell expressions. From Eq. (5) it is clear that the optimal $\lambda_i$ corresponds to the eigenvector belonging to the largest eigenvalue of the matrix

$$ \sum_{\mu=0}^{m_A} \sum_{\nu=0}^{m_B} M_{\mu\nu} A_{ij}^\mu B_{ij}^\nu, $$

and the eigenvalue is just the value of the Bell expression. It is not sure that the components of the largest eigenvector will all be positive real numbers. If they are not, they can not be called Schmidt coefficients. However, this does not affect anything, it is best just to leave them as they are. If we want to see the final result for the state vector represented by its Schmidt coefficients, it is enough to make the appropriate transformation at the end of the calculation. We simply have to multiply rows and columns of either Alice’s or Bob’s matrices with phase factors.

The algorithm consists of repeating these three steps until the value of the Bell expression reach convergency. As this number may only increase in each step, convergence is ensured. What is not ensured is that we will converge to the global optimum of the problem. Therefore, we have to repeat the full procedure many times with different initial values. We may save computation time if we stop a run when it clearly goes towards an inferior solution. For example, if we are interested in a solution belonging to a larger Hilbert space, we may stop whenever too many components of the state vector falls below some threshold.

It is not difficult to extend the method to more than two participants. In that case there is no Schmidt decomposition, which would ensure that one can choose the bases in the component spaces such that the $n^2$-dimensional state vector has only $n$ nonzero components. However, one can still use Eq. (6) to calculate the optimum measurement operators for Alice, and analogous equations for the operators of the other participants. The only difference is that the formula for the matrix of $\hat{X}_\mu$ (and the corresponding matrices for the other participants) will be somewhat more complicated than Eq. (7), involving summations to more indices. The optimum state vector can also be calculated as the eigenvector belonging to the largest eigenvalue of a matrix, but this will be a more general matrix in the full $n^2$-dimensional
Hilbert space. As the third step of the algorithm in this case involves the diagonalization of a much larger matrix than the first two steps, it is more efficient to do it less frequently, that is to repeat the first and the second steps several times before updating the state vector.

III. FAMILY OF CONSTRUCTIONS

From the optimality of formula (5) it follows that the matrices of the optimum \( \hat{A}_1, \hat{A}_2, \hat{A}_3, \hat{B}_1, \hat{B}_2 \) and \( \hat{B}_3 \) are such that they satisfy the following Eq. (9), Eq. (10), Eq. (11), Eq. (12), Eq. (13) and Eq. (14), respectively:

\[
\sum_{i,j=1}^{n} A_{ij}^1 (B_{ij}^1 + B_{ij}^2 - B_{ij}^3) \lambda_i \lambda_j = \max \quad (9)
\]

\[
\sum_{i,j=1}^{n} A_{ij}^2 (B_{ij}^1 + B_{ij}^2 - B_{ij}^3) \lambda_i \lambda_j = \max \quad (10)
\]

\[
\sum_{i,j=1}^{n} A_{ij}^3 (B_{ij}^2 - B_{ij}^1) \lambda_i \lambda_j = \max \quad (11)
\]

\[
\sum_{i,j=1}^{n} B_{ij}^1 (A_{ij}^1 + A_{ij}^2 - A_{ij}^3) \lambda_i \lambda_j = \max \quad (12)
\]

\[
\sum_{i,j=1}^{n} B_{ij}^2 (A_{ij}^1 + A_{ij}^2 + A_{ij}^3 - 2 \delta_{ij}) \lambda_i \lambda_j = \max \quad (13)
\]

\[
\sum_{i,j=1}^{n} B_{ij}^3 (A_{ij}^2 - A_{ij}^1) \lambda_i \lambda_j = \max \quad (14)
\]

Meanwhile, \( \lambda_i \) are the components of the eigenvector belonging to the maximum eigenvalue of the matrix

\[
M_{ij} = -(A_{ij}^2 + B_{ij}^1 + 2B_{ij}^2) \delta_{ij} + (A_{ij}^1 + A_{ij}^2)(B_{ij}^1 + B_{ij}^2) + A_{ij}^3 (B_{ij}^2 - B_{ij}^1) + B_{ij}^3 (A_{ij}^2 - A_{ij}^1). \quad (15)
\]

The matrix of the measurement operators we got with \( \sum_{i,j=1}^{n} A_{ij}^1 (B_{ij}^1 + B_{ij}^2 - B_{ij}^3) \lambda_i \lambda_j = \max \) may be written as

\[
\hat{A}_2 = \begin{pmatrix}
1 & \frac{1-c_s}{2} & \frac{s_3}{2} & \frac{1-c_s}{2} & \frac{s_3}{2} \\
\frac{1-c_s}{2} & \frac{1-c_s}{2} & \frac{s_3}{2} & \frac{1-c_s}{2} & \frac{s_3}{2} \\
\frac{s_3}{2} & \frac{1-c_s}{2} & \frac{1-c_s}{2} & \frac{1-c_s}{2} & \frac{s_3}{2} \\
\frac{s_3}{2} & \frac{1-c_s}{2} & \frac{1-c_s}{2} & \frac{1-c_s}{2} & \frac{s_3}{2} \\
\frac{s_3}{2} & \frac{1-c_s}{2} & \frac{1-c_s}{2} & \frac{1-c_s}{2} & \frac{s_3}{2}
\end{pmatrix},
\]

with \( s_i = \sqrt{1-c_i^2} \) are all positive. The matrix of \( \hat{A}_1 \) turns out to be the same, but the offdiagonal elements have a negative sign. The form of \( \hat{B}_2 \) is the following:

\[
\hat{B}_2 = \begin{pmatrix}
\frac{1+c_s}{2} & \frac{s_1}{2} & \frac{1+c_s}{2} & \frac{s_3}{2} & \frac{1+c_s}{2} \\
\frac{s_1}{2} & \frac{1+c_s}{2} & \frac{1+c_s}{2} & \frac{s_3}{2} & \frac{1+c_s}{2} \\
\frac{1+c_s}{2} & \frac{s_3}{2} & \frac{1+c_s}{2} & \frac{s_3}{2} & \frac{1+c_s}{2} \\
\frac{s_3}{2} & \frac{1+c_s}{2} & \frac{s_3}{2} & \frac{1+c_s}{2} & \frac{s_3}{2} \\
\frac{s_3}{2} & \frac{1+c_s}{2} & \frac{s_3}{2} & \frac{s_3}{2} & \frac{1+c_s}{2}
\end{pmatrix},
\]

The matrix element \( B_{nn}^2 \) may take the value of 1 and 0, when \( c_n = 0 \) and \( c_n = -1 \), respectively. For smaller dimensions we got the former value for all best solutions, but it turned out that from dimensions larger than \( n = 79 \) the other value gives the better solution. The notation of \( B_{nn}^2 = 1 + c_n \) will become clear later. The matrix of \( \hat{B}_1 \) is the same as that of \( \hat{B}_2 \), but \( B_{nn}^1 = 0 \), and like in the case of \( \hat{A}_1 \), the offdiagonal matrix elements are negative. Matrices \( \hat{A}_3 \) and \( \hat{B}_3 \) have even simpler forms:

\[
A_{nn}^3 = B_{nn}^3 = 1, \quad \text{while all elements of the two by two blocks are 1/2.}
\]

It is easy to check that if all \( \lambda_i > 0 \), then the matrices of \( \hat{A}_3 \) and \( \hat{B}_3 \) do satisfy the optimality conditions Eq. (11) and Eq. (14), respectively. The matrix of \( \hat{A}_3 \) has the same block structure as \( \hat{B}_2 - \hat{B}_1 \), as it should, and the optimality condition can be checked block by block. The value of the single element block in the matrix of \( \hat{B}_2 - \hat{B}_1 \), that is \( B_{nn}^2 - B_{nn}^1 \) is either 2 or 0, depending on \( c_n \), in the first case the optimum is \( A_{nn}^3 = 1 \), while in the other case the chosen value 1 is just as good as value 0 would have been. The two by two blocks in the matrix of \( B_{nn}^2 - B_{nn}^1 \) have zero diagonal elements, and positive nondiagonal elements. As all \( \lambda_i \) have the same sign, the number they will be multiplied with is also positive. Therefore, the optimum two by two block of the matrix of \( \hat{A}_3 \) is the symmetric two-dimensional matrix with eigenvalues 0 and 1 having the largest possible nondiagonal elements. This matrix is the one whose all four elements are 1/2.

From Eq. (16) we can get equations determining the parameters of the matrix of \( \hat{A}_2 \) that is \( c_i \) with \( i \) even (see Eq. (16)) in terms of the parameters of the matrices of Bob’s measurement operators, that is \( c_i \) with \( i \) odd, and
the Schmidt coefficients $\lambda_i$. As the matrix of $\hat{B}_1 + \hat{B}_2 - \hat{I}$ is diagonal, the block structure of $\hat{A}_1$ is the same as that of $\hat{B}_3$. The matrix of $\hat{B}_1 + \hat{B}_2 + \hat{B}_3 - \hat{I}$ is:

$$
\hat{B}_1 + \hat{B}_2 + \hat{B}_3 - \hat{I} = 
\begin{pmatrix}
    c_1 & \frac{1}{2} - c_1 & \frac{1}{2} & \frac{1}{2} + c_3 \\
    \frac{1}{2} - c_1 & 1 - c_1 & \frac{1}{2} & \frac{1}{2} + c_5 \\
    \frac{1}{2} & \frac{1}{2} - c_1 & \frac{1}{2} - c_2 & \frac{1}{2} + c_5 \\
    \frac{1}{2} & \frac{1}{2} & \frac{1}{2} - c_2 & \frac{1}{2} + c_5 \\
    \vdots & \vdots & \vdots & \vdots \\
    \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} + c_n \\
\end{pmatrix}
$$

(18)

The value of $A^2_{11}$ is determined by the sign of $c_1$, the $A^2_{11} = 1$ value is correct if $c_1 > 0$, which turns out to be true. Each $c_i$, where $i$ is even, occurs only in one two by two block of the matrix of $\hat{A}_2$ (see Eq. (16)). Its optimum value depends on the corresponding block in Eq. (18), containing $c_{i-1}$ and $c_{i+1}$. We denoted $B^2_{nn}$ as $1 + c_n$ such that the last block has the same form as the others. Using Eq. (10) we arrive at the equation determining the optimum value of $c_i$:

$$
\frac{(1 - c_i)}{2} \left( \frac{1 - c_{i-1}}{2} \right) \lambda_i^2 - \frac{(1 + c_i)}{2} \left( \frac{1}{2} + c_{i+1} \right) \lambda_{i+1}^2 + \frac{s_i}{2} \lambda_i \lambda_{i+1} = \max
$$

(19)

Multiplying the equation by four, dropping terms constant in $c_i$ and substituting $s_i = \sqrt{1 - c_i^2}$ we get:

$$
c_i \left[ (1 + 2c_{i+1})\lambda_{i+1}^2 - (1 - 2c_{i-1})\lambda_i^2 \right] + 2\sqrt{1 - c_i^2} \lambda_i \lambda_{i+1}
= \max
$$

(20)

from which it follows that

$$
c_i = \frac{\tau_i}{\sqrt{\tau_i^2 + 4\lambda_i^2 \lambda_{i+1}^2}},
$$

(21)

where

$$
\tau_i \equiv (1 + 2c_{i+1})\lambda_{i+1}^2 - (1 - 2c_{i-1})\lambda_i^2.
$$

(22)

With $c_i$ chosen this way Eq. (19), the optimality condition for $\hat{A}_1$ is also satisfied. If we started from this condition instead of the one for $\hat{A}_2$, we would have arrived at exactly the same results.

In the same way as above, from Eq. (12) and Eq. (13) we can derive formulae for the optimum values of the parameters of the matrices of $\hat{B}_1$ and $\hat{B}_2$, that is for $c_i$, where $i$ is odd. These formulae turn out to have exactly the same form as the ones derived for even $i$ values, that is Eqs. (19,22) are valid for odd $i$. To get $c_1$, we have to introduce the notation $c_0 \equiv 1$. The value $B^2_{1n} = 0$ is the optimum value. Either $B^2_{2n} = 0$ (that is $c_n = -1$) or $B^2_{2n} = 1$ (that is $c_n = 0$) is a possible choice. Consistency with the optimality condition is fulfilled if $c_{n-1} \leq 0$ in the first case, and $c_{n-1} \geq 0$ in the second one.

With the specific forms of the measurement operators above, the matrix $M$ of Eq. (13), whose eigenvector corresponding to its largest eigenvalue gives the Schmidt coefficients $\lambda_i$, is tridiagonal, and its nonzero matrix elements are:

$$
M_{ii} = c_{i-1} c_i + \frac{c_{i-1} - c_i}{2} + \frac{c_n + 1}{2} \delta_{in},
$$

$$
M_{i(i+1)} = \frac{s_i}{2}.
$$

(23)

We may apply the iterative method with confining ourselves to the present specific forms of the operators, and get solutions for very large dimensions. This way we may increase the dimensionality of the component Hilbert spaces even to a thousand, or more. The distance of the maximum value of the Bell expression from the upper bound $0.25087538$ calculated at level four is shown in Fig. 1 as a function of the dimensionality, both for $c_n = 0$ and $c_n = -1$. For lower dimensions the former family of solutions is much better. Still, even this gives a value larger than 0.25, which one can obtain with a pair of real qubits only if $n \geq 12$. Unfortunately, this family does not converge to the upper bound. The other family with $c_n = -1$ is initially inferior, but above $n = 79$ it overtakes the other one, and converges to $0.250875384514$, a value well consistent with the upper bound: it is slightly larger, but within the numerical accuracy of the bound. In Fig. 2 and Fig. 3 we show $\lambda_i$ and $c_i$ for $n = 99$ with $c_n = 0$ and $c_n = -1$, respectively. For small $i$ the $c_i$ is close to $c_0=0$, and tends to a constant value fast. In the case of $c_n = 0$ it stays basically constant up to the last few point, when it drops towards the zero value of $c_n$ fast. When $c_n = -1$ and $n > 19$ there are more than one solutions. In all solutions $c_i > 0$ for small $i$ and $c_i < 0$ for
large $i$. In the different solutions the change of sign happens between two neighbouring integers. For very large $n$ it always happens above 16 and below $n - 16$. Among all these solutions the best is the one in which $c_i$ changes sign exactly in the middle, that is between $(n - 1)/2$ and $(n + 1)/2$. In Fig. 3 we show the result for this solution. In particular, the upper curve in Fig. 3 shows the behaviour of $c_i$. The curve starts like in the case of $c_n = 0$, that is it drops from $c_0 = 1$ to a constant value fast, that stays there until it goes to minus one times the constant value in a relatively short interval, and then it stays almost constant again until it turns towards $c_n = -1$ at the end. Where $c_i$ is constant, $\lambda_i$ behaves exponentially.

Knowing the behaviour of $c_i$, it is easy to choose initial values such that the iterative procedure will converge to the desired solution for the first time, there is no need for repeated runs. For example, we may initialize $c_i$ as $+C$ for $i < n/2$ and $-C$ for $i > n/2$, with $C = 0.9$. Then we can start with the third step instead of the first one, that is with the determination of $\lambda_i$.

The families of solutions may be extended to even values of $n$. The matrices of the measurement operators are blockdiagonal, like for odd $n$. The matrices of $B_1$, $B_2$ and $A_3$ consist of $n/2$ two by two blocks. The blocks of $A_1$, $A_2$ and $B_3$ are also two-dimensional except for the first and the last ones, which have single elements. The actual form of the matrices can be parametrized with $c_i$ analogously to the odd $n$ case, which will satisfy the same equations as optimality conditions, and the eigenvalue equation for $\lambda_i$ will also have the same form. Figure 1 does contain the results for $n$ even. The curve for $c_i$ in the case of the best solution with $c_n = -1$ is not fully symmetric. It changes either very nearly half way between $n/2 - 1$ and $n/2$ or between $n/2$ and $n/2 + 1$. If we make the change of size to happen at the middle, that is we enforce $c_{n/2} = 0$, for large $n$ the result will converge to the same suboptimal value as in the case of the $c_n = 0$ family. Probably the reason this family fails to converge to the true optimum is that $c_i$ must approach zero at an integer value, instead of midway between two integers.

In the matrices of the measurement operators we made very specific choices for the values of the single element blocks, leaving only $c_n$ as a single free parameter. We note that there are other choices consistent with the optimality conditions, but they lead to solutions equivalent with the ones discussed.

**IV. OTHER EXAMPLES**

In Ref. [13] we calculated both lower and upper bounds for all known tight binary bipartite Bell inequalities with up to five measurement settings per party. For most cases we managed to find explicit solutions saturating the upper bound. There were 20 exceptions. The case of $I_{3222}$ was discussed in the previous chapter. Now we have applied the iterative algorithm with up to 25 dimensional component spaces for the remaining 19 problems. In 11 cases we have found better solution than the ones we reported in Ref. [13]. The solution for $A_{65}$ could have been found by our previous methods, but we missed it. All the other ones involve larger Hilbert spaces than those methods could handle. We have also made the upper bound tighter by going to higher levels by using a computer with larger memory. As previously, the calculations have been done with Borcher’s code CSDP for semidefinite programming [30]. For cases with five measurement settings per party we could do the calculation on level two plus $aa^i b$ plus $ab^i$. For the smaller cases we could afford to go up to level three, except for $I_{3222}$, where we did level four. The notion of levels and partial levels, and their notation is explained in Ref. [11], and also in Ref. [13]. This
way the two bounds met for $A_{65}$. We sent $A_{67}$ at level three, and $J_{4422}^{33}$ and $J_{4422}^{48}$ at level three plus $aa'bb'$ to Brian Borchers, as test cases for his new code which requires much less memory than CSDP for very large cases. For $A_{67}$ this new upper bound does agree with the lower one. Unfortunately, for $J_{4422}^{48}$ there remained a difference of 0.000012, significantly less than the level three value of 0.0000657, but more than numerical uncertainty. At an even higher level it would probably disappear, but it is not sure. Therefore, we can not state that our solution with 12-dimensional component spaces is already the optimum one. The case $J_{4422}^{33}$ at level three plus $aa'bb'$ seems to be a difficult case for the new code, it could solve it only at a reduced accuracy, and the value it has given for the upper bound turned out to be lower than the lower bound. Therefore, very probably the solution with a pair of real qubits we found the best so far is actually the optimum. If we added to level three just one quarter of the $aa'bb'$ type terms, we could use CSDP. In the cases of $I_{32}^{32}$ and $J_{4422}^{33}$ this was already enough to reach the lower bound. By looking at the dependence of the upper bound on the level it has been calculated, we are almost sure that for $J_{4422}^{30}$, $J_{4422}^{48}$, $A_{47}$, $A_{42}$, $A_{64}$, $A_{62}$ and $A_{80}$ the present lower bound will not be reached, therefore we do not yet have the optimum solution. Probably $I_{32}^{32}$ is not the only inequality requiring infinite dimensional Hilbert spaces for maximum violation. Actually, the difference in the cases of $J_{4422}^{33}$ and $A_{82}$ is very small, but it does not change much with increasing level. For $A_{80}$ and $A_{84}$ the upper bound would more probably converge to our solution, while for the rest of the cases we can not tell from the present results.

Bancal et al. [25] found recently two symmetric inequalities with four settings per party, which they called $S_{51}$ and $S_{52}$. They were also included in our calculations. In fact, both of them could be saturated with measurements acting on qubits, we found the maximum violation to be 1.0135274 and 0.87038004 for $S_{51}$ and $S_{52}$, respectively.

The details of our best solutions, including Schmidt coefficients and the matrices of the measurement operators are on our web site [20].

V. CONCLUSION

To summarize, we investigated the $I_{32}^{32}$ Bell inequality and its maximal quantum violation. Although $I_{32}^{32}$ is one of the simplest Bell inequalities with just three measurements per party, surprisingly we found that the maximum value of 0.25 achievable with a pair of qubits could be only be overcome by using states of dimension at least $12 \times 12$. Moreover, we found a family of measurement operators and states, which attains numerically in very large dimensional Hilbert spaces (and hence in the limit of infinite dimensions as well) the largest possible

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TABLE I: Results for the 19 Bell inequalities for which the tightness of the quantum bound has not been proven. The local Hilbert space necessary to achieve the best lower bound is denoted by $H$, column 'New' tells if this lower bound is an improvement over our previous result, and column 'Level' is the level to derive the upper bound.

| Case | Lower bound | $H$ | New | Upper bound | Level |
|------|-------------|-----|-----|-------------|-------|
| $J_{4422}^{30}$ | 0.4676794 | $\mathbb{R}^4$ | no | 0.0000000 | $L3 + aa'bb'$ |
| $J_{4422}^{30}$ | 0.4363842 | $\mathbb{R}_{17}^4$ | yes | 0.0008787 | $L3$ |
| $J_{4422}^{44}$ | 0.4492657 | $\mathbb{R}^4$ | no | 0.0000000 | $L3 + aa'bb'$ |
| $J_{4422}^{48}$ | 0.7516220 | $\mathbb{R}_{12}^4$ | no | 0.0001200 | $L3 + aa'bb'$ |
| $J_{4422}^{52}$ | 0.7500755 | $\mathbb{R}^6$ | no | 0.0000166 | $L3$ |
| $J_{4422}^{53}$ | 1.1223170 | $\mathbb{R}_{20}^4$ | yes | 0.0002409 | $L3$ |
| $J_{4422}^{57}$ | 1.1583626 | $\mathbb{R}^2$ | no | 0.0001425 | $L3$ |
| $A_{14}$ | 0.4759513 | $\mathbb{R}_{20}^4$ | yes | 0.0018953 | $L3$ |
| $A_{21}$ | 0.3260601 | $\mathbb{R}_{10}^4$ | yes | 0.0001176 | $L3$ |
| $A_{47}$ | 0.4608544 | $\mathbb{C}^2$ | no | 0.0020847 | $L2 + aa'bb'$ |
| $A_{62}$ | 0.4065268 | $\mathbb{R}_{15}^4$ | yes | 0.0003457 | $L2 + aa'bb'$ |
| $A_{64}$ | 0.3900989 | $\mathbb{R}^4$ | no | 0.0013878 | $L2 + aa'bb'$ |
| $A_{65}$ | 0.3688996 | $\mathbb{R}^5$ | yes | 0.0000000 | $L2 + aa'bb'$ |
| $A_{67}$ | 0.3990671 | $\mathbb{R}^5$ | no | 0.0000000 | $L3$ |
| $A_{68}$ | 0.4025522 | $\mathbb{R}_{18}^4$ | yes | 0.0052407 | $L2 + aa'bb'$ |
| $A_{80}$ | 0.3769863 | $\mathbb{R}^4$ | no | 0.0002557 | $L2 + aa'bb'$ |
| $A_{82}$ | 0.4708838 | $\mathbb{R}_{20}^4$ | yes | 0.0003410 | $L2 + aa'bb'$ |
| $A_{84}$ | 0.6352087 | $\mathbb{R}_{18}^4$ | yes | 0.0007476 | $L2 + aa'bb'$ |
| $A_{89}$ | 0.3035637 | $\mathbb{R}_{17}^4$ | yes | 0.0022575 | $L2 + aa'bb'$ |
value of the Bell expression $I_{3322}$ allowed by quantum theory. Taking as a conjecture that our construction is optimal (in the sense that no finite dimension suffices to achieve the true quantum maximum for $I_{3322}$), to our knowledge this constitutes the first example of a Bell scenario concerning finite number of measurements and outcomes, where measuring finite dimensional quantum systems is not enough to obtain exactly all quantum correlations. In this respect we wish to invoke the concept of dimension witnesses introduced recently in Ref. [30]. In a broader sense, the aim of this concept is to put a lower bound on the Hilbert space dimension needed to reproduce the statistics arising from a Bell experiment. Dimension witnesses have been found or conjectured in many different scenarios, such as for the bipartite setting [13, 14, 17, 31–33] for the multipartite setting [34] and even for the case of a single system [35].

In particular, for measurements with binary outcomes it was shown how to get dimension witnesses analytically for any dimensions [31]. Actually, these results entail that no finite dimension is sufficient to generate the whole set of quantum correlations provided an arbitrary number of two-outcome measurements is involved. Consider now a scenario where the number of measurements (each having a finite number of outcomes) is finite. Does there exist a Bell inequality requiring infinitely large entangled states for obtaining the maximum possible quantum violation? That is, are there quantum correlations corresponding to this scheme attainable exactly by measuring infinite dimensional quantum systems? This is a question posed recently by Navascués et al. [11].

Indeed, in the present paper we suggested, supported by thorough numerical computations, that no finite dimension suffices to maximally violate the $I_{3322}$ inequality. While we cannot guarantee that for any finite dimension there exist no other construction beyond ours giving a larger quantum value, nevertheless we showed that our best conjectured values tend to the upper limit computed with the aid of the NPA method [10]. We pose it as a challenge to provide an analytical proof of our conjecture. Also, in our view it would be interesting to find other, bipartite or multipartite, Bell inequalities beyond $I_{3322}$ (but still involving finite number of settings and outcomes) requiring infinitely large entangled states for their maximal quantum violation.

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