Bounding Temporal Quantum Correlations

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Sequential measurements on a single particle play an important role in fundamental tests of quantum mechanics. We provide a general method to analyze temporal quantum correlations, which allows us to compute the maximal correlations for sequential measurements in quantum mechanics. As an application, we present the full characterization of temporal correlations in the simplest Leggett-Garg scenario and in the sequential measurement scenario associated with the most fundamental proof of the Kochen-Specker theorem.

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Introduction.—The physics of microscopic systems is governed by the laws of quantum mechanics and exhibits many features that are absent in the classical world. The best-known result showing such a difference is due to Bell [1]. The assumptions of realism and locality lead to bounds on the correlations—the Bell inequalities, and these bounds are violated in quantum mechanics. Interestingly, this quantum violation is limited for many Bell inequalities and does not reach the maximal possible value. For instance, the Bell inequality derived by Clauser, Horne, Shimony, and Holt (CHSH) bounds the correlation [2]

\[ B = \langle A_1 \otimes B_1 \rangle + \langle A_1 \otimes B_2 \rangle + \langle A_2 \otimes B_1 \rangle - \langle A_2 \otimes B_2 \rangle, \tag{1} \]

where \(A_i\) and \(B_j\) are measurements on two different particles. On the one hand, local realistic models obey the CHSH inequality \(B \leq 2\), which is violated in quantum mechanics. On the other hand, the maximal quantum value is upper bounded by \(B \leq 2\sqrt{2}\), a result known as Tsirelson’s bound [3]. Whereas this bound holds within quantum mechanics, it has turned out that hypothetical theories that reach the algebraic maximum \(B = 4\) without allowing faster-than-light communication are possible [4]. This raises the question of whether the bounded quantum value can be derived on physical grounds from fundamental principles. Partial results are available, and principles have been suggested that bound the correlations: in a world where maximal correlations are observed, the communication complexity is trivial [5], a principle established as information causality is trivial [6], and there exists no reversible dynamics [7].

The question of how and why quantum correlations are fundamentally limited has been discussed mainly in the scenario of bipartite and multipartite measurements. What happens, however, if we shift the attention from spatially separated measurements to temporally ordered measurements? There is no need to measure on distinct systems as in Eq. (1), but rather, we may perform sequential measurements on the same system. Then, an elementary property of quantum mechanics becomes important: the measurement changes the state of the system. In fact, this allows us to temporally “transmit” a certain amount of information [8], and one would expect that the correlations in the temporal case can be larger than in the spatial situation.

We stress that sequential measurements also have been considered in the analysis of the question how quantum and classical mechanics are different, the most well-established results here are quantum contextuality (the Kochen-Specker theorem [9]) and macrorealism (Leggett-Garg inequalities [10]); cf. Fig. 1. The research in this fields has triggered experiments involving sequential measurements. For demonstrating such a contradiction between classical and quantum physics, e.g., the correlation

\[ S_5 = \langle A_1 A_2 \rangle_{\text{seq}} + \langle A_2 A_3 \rangle_{\text{seq}} + \langle A_3 A_4 \rangle_{\text{seq}} + \langle A_4 A_5 \rangle_{\text{seq}} - \langle A_5 A_1 \rangle_{\text{seq}}, \tag{2} \]

has been considered [11] [12]. Here, \(\langle A_i A_j \rangle_{\text{seq}}\) denotes a sequential expectation value that is the average of the product of the value of the observables \(A_i\) and \(A_j\) when first \(A_i\) is measured, and afterwards \(A_j\). One can show that for macrorealistic theories as well as for noncontextual models the bound \(S_5 \leq 3\) holds, but in quantum mechanics, this can be violated.

Here however, we are rather interested in the fundamental bounds on the temporal quantum correlations, with no assumption about the compatibility of the observables. Special cases of this problem have been discussed before: for Leggett-Garg inequalities, maximal values for two-level systems have been derived [11] [13], and temporal inequalities similar to the CHSH inequality have been discussed [8] [14].

We provide a method that allows us to compute the maximal achievable quantum value for an arbitrary inequality and thus we solve the problem of bounding temporal quantum correlations. First, we will discuss a simple method, which can be used for expressions as in Eq. (2), where only sequences of two measurements are considered. Then, we introduce a general method which can be used for arbitrary sequential measurements, resulting in a complete characterization of the possible
quantum values. Interestingly, our methods characterize temporal correlations exactly, whereas for the case of spatially separated measurements only converging approximations are known.

**Projective measurements.**—When determining the maximal value for sequential measurements as in Eq. (2) we consider projective measurements, as these are the standard textbook examples of quantum measurements. The underlying formalism has been established by von Neumann [15] and Lüders [16]. An observable \( A \) with possible results \( \pm 1 \) is described by two projectors \( \Pi_+ \) and \( \Pi_- \) such that \( A = \Pi_+ - \Pi_- \). If the observable \( A \) is measured, the quantum state is projected onto the space of the observed result, i.e., \( \rho \mapsto \Pi_+ \rho \Pi_+ / \text{Tr}(\rho \Pi_+) \). Applying this scheme to the case of sequential measurements, one finds that the sequential mean value can be written as

\[
\langle A_i A_j \rangle_{\text{seq}} = \frac{1}{2} [\text{Tr}(\rho A_i A_j) + \text{Tr}(\rho A_j A_i)].
\]

It is interesting to notice that for pairs of \( \pm 1 \)-valued observables such a mean value does not depend on the order of the measurement [8].

**The simplified method.**—We first show how the maximal quantum mechanical value for an expression such as \( S_5 \) in Eq. (5) can be determined. First, we consider a set \( \mathcal{A} = \{ A_i \} \) of \( \pm 1 \)-valued observables and a general expression \( C = \sum_{ij} \lambda_{ij} \langle A_i A_j \rangle_{\text{seq}} \). The correlations given in Eq. (2) are just a special case of this scenario. Then, we consider the matrix built up by the sequential mean values \( X_{ij} = \langle A_i A_j \rangle_{\text{seq}} \). This matrix has the following properties: (i) it is real and symmetric, \( X = X^T \), (ii) the diagonal elements equal one, \( X_{ii} = 1 \), and (iii) the matrix has no negative eigenvalue (or \( v^T X v \geq 0 \) for any vector \( v \)), denoted as \( X \succeq 0 \) (see Appendix A2). A similar construction for the matrix \( X \), together with the optimization problem below, has been considered before in relation with Bell inequalities [17]. However, our method involves a different notion of correlations, namely that given by Eq. (3).

The main idea is now to optimize the expression \( C = \sum_{ij} \lambda_{ij} X_{ij} \) over all matrices with the properties (i)–(iii) above. Hence, we consider the optimization problem

\[
\text{maximize: } \sum_{ij} \lambda_{ij} X_{ij}, \quad (4)
\]

subjected to: \( X = X^T \succeq 0 \) and for all \( i, X_{ii} = 1 \).

Since all matrices \( X \) that can originate from a sequence of quantum measurements will be of this form, one performs the optimization over a potentially larger set. Thus, the solution of this optimization is, in principle, just an upper bound on the maximal quantum value of \( S_5 \). Note that the optimization itself can be done efficiently and is assured to reach the global optimum since it represents a so-called semidefinite program [18]. In the case of \( S_5 \), this optimization can even be solved analytically and gives

\[
S_5 \leq \frac{5}{4} \left( 1 + \sqrt{5} \right) \approx 4.04. \quad (5)
\]
It turns out that appropriately chosen measurements on a qubit already reach this value (see Appendix A2 and Refs. [19])2]. Hence, this upper bound is tight. More generally, one can prove that each matrix $X$ with the above properties has a sequential quantum representation (see Appendix A2). Finally, note that if the observables in each sequence are required to commute, then the maximal quantum value for $S_5$ is known to be $\Omega_{QM} = 4\sqrt{5} - 5 \approx 3.94$ [20, 21].

The general method.—The above method can only be used for correlations terms of sequences of at most two $\pm 1$-valued observables. In the following, we discuss the conditions allowing a given probability distribution to be realized as sequences of measurements on a single quantum system in the general setting. We label as $r = (r_1, r_2, \ldots, r_n)$ the results of an $n$-length sequence obtained by using the setting $s = (s_1, s_2, \ldots, s_n)$. The ordering is such that $r_1, s_1$ label the result and the setting for the first measurement etc. The outcomes of any such sequence are sampled from the sequential conditional probability distribution

\[ P(r|s) \equiv P_{seq}(r_1, r_2, \ldots, r_n|s_1, s_2, \ldots, s_n). \] (6)

In the case of projective quantum measurements, each individual result $r$ of any setting $s$ is associated with a projector $\Pi_r$, which altogether satisfy two requirements: for each setting the operators must sum up to the identity, i.e., $\sum_r \Pi_r = I$ and they satisfy the orthogonality relations $\Pi_r \Pi_{r'} = \delta_{r,r'} \Pi_r$, where $\delta_{r,r'}$ is the Kronecker symbol. Finally, after the measurement with the setting $s$ and result $r$, the quantum state is transformed according to the rule $\varrho \rightarrow \Pi_r \varrho \Pi_r^\dagger / P(r|s).

In the following, we say that the conditional probability distribution $P(r|s)$ has a sequential projective quantum representation if there exists a suitable set of such operators $\Pi_r$ and an appropriate initial state $\varrho$ such that

\[ P(r|s) = \text{Tr}[\Pi(r|s)\Pi(r|s)^\dagger \varrho], \] (7)

with the shorthand $\Pi(r|s) = \Pi_{r_1} \Pi_{r_2} \cdots \Pi_{r_n}$.

Whether a given distribution $P(r|s)$ indeed has such a representation can be answered via a so-called matrix of moments, which often appears in moment problems [17, 22, 24]. This matrix, denoted as $M$ in the following, contains the expectation value of the products of the above-used operators $\Pi(r|s)$ at the respective position in the matrix. In order to identify this position we use as a label the abstract operator sequence $r|s$ for both row and column index. In this way the matrix is defined as

\[ M_{r|s,r'|s'} = \langle \Pi(r|s)\Pi(r'|s') \rangle. \] (8)

Whenever this matrix is indeed given by a sequential projective quantum representation, the matrix $M$ satisfies two conditions: (a) linear relations of the form $M_{r|s,r'|s'} = M_{r'|s',r|s}$ if the underlying operators are equal as a consequence of the properties of normalization and orthogonality of projectors, (b) $M \geq 0$ since $v^\dagger M v \geq 0$ holds for any vector $v$, because such a product can be written as the expectation value $\langle C C^\dagger \rangle_{\varrho} \geq 0$ which is non-negative for any operator $C$. Finally, note that certain entries of this matrix are the given probability distribution, for instance, at the diagonal $M_{r=s|r=s} = P(r|s)$. The main point, however, is the converse statement: given a moment matrix with properties (a) and (b) above, the associated probability distribution $P(r|s)$ always has a sequential projective quantum representation (see Appendix A3).

Hence, the search for quantum bounds represents again a semidefinite program. The fact that this characterization is sufficient is in stark contrast with the analogue technique in the spatial Bell-type scenario [22, 23], where one needs to use moment matrices of an increasing size $n$ to generate better superset characterizations which only become sufficient in the limit $n \to \infty$. However, indirectly, the sufficiency of our method has already been proven in this context [23] (see Appendix A3).

Applications.—To demonstrate the effectiveness of our approach, we discuss four examples. First, we consider the original Leggett-Garg inequality

\[ S = \langle M(t_1)M(t_2) \rangle_{seq} + \langle M(t_2)M(t_3) \rangle_{seq} - \langle M(t_1)M(t_2) \rangle_{seq} \leq 1. \] (9)
This bound holds for macrorealistic models, and it has been shown that in quantum mechanics values up to $S = 3/2$ can be observed \[10, 11, 13\]. Our methods allow us not only to prove that this value is optimal for any dimension and any measurement, but also to, for instance, determine all values in the three-dimensional space of temporal correlations $\langle M(t_i)M(t_j) \rangle$, which can originate from quantum mechanics. The detailed description is given in Fig. 2, and the calculations are given in the Appendix A1.

Second, we consider generalizations of the Eq. (2) with a larger number of measurements, known as $N$-cycle inequality \[20, 21\].

$$S_N = \sum_{i=0}^{N-2} \langle A_iA_{i+1} \rangle_{\text{seq}} - \langle A_{N-1}A_0 \rangle_{\text{seq}}. \quad (10)$$

For this case, everything can be solved analytically (see Appendix A2) leading to the bound

$$S_N \leq N \cos \left( \frac{\pi}{N} \right), \quad (11)$$

which can be reached by suitably chosen measurements. This value has already occurred in the literature \[11, 19\], but only qubits have been considered. Our proof shows that it is valid in arbitrary dimension. Note that the fact that the maximal value is obtained on a qubit system is not trivial, although the measurements are dichotomic. For Kochen-Specker inequalities with dichotomic measurements examples are known, where the maximum value cannot be attained in a two-dimensional system \[19\] and also for Bell inequalities this has been observed \[20, 27\].

As a third application, we consider the noncontextuality scenario recently discovered by S. Yu and C. H. Oh \[28\]. There, thirteen measurements on a three-dimensional system are considered, and a noncontextuality inequality is constructed, which is violated by any quantum state. It has been shown that this scenario is the simplest situation where state-independent contextuality can be observed \[29\], so it is of fundamental importance. We can directly apply our method to the original inequality by Yu and Oh, as well as recent improvements \[30\] and compute the corresponding Tsirelson-like bounds. We recall that our results are not directly related to the phenomenon of quantum contextuality, since no compatibility of the measurements is assumed, but they show the effectiveness of our method even on complex scenarios, namely, inequalities containing 37 or 41 terms, that involve sequential measurements. Our results are summarized in Table 1.

Another class of inequalities is given by the guess-your-neighbor’s-input inequalities \[31\], which if viewed as multipartite inequalities, show no quantum violation but a violation with the use of postquantum no-signalling resources. We calculate the sequential bound for the case of measurement sequences of length three, instead of measurement on three parties. We consider

$$P(000|000) + P(110|011) + P(011|101) + P(101|110) \leq \Omega_{C,Q} \leq \Omega_S \leq \Omega_{NS}, \quad (12)$$

with the notation $P(r_1,r_2,r_3|s_1,s_2,s_3)$ as before, and possible results and settings $r_i \in \{0,1\}$ and $s_i \in \{0,1\}$. We find that

$$\Omega_S \approx 1.0225, \quad (13)$$

while it is known that $\Omega_{C,Q} = 1$ and $\Omega_{NS} = \frac{4}{3}$, where the indices $C,Q,S,NS$ label, respectively, the classical, quantum, sequential and no-signalling bounds. So, in this case, the bound for sequential measurements is higher than the bound for spatially separated measurements. This also highlights the greater generality of our method in comparison with the results of Ref. \[8\]: there, only temporal inequalities with sequences of length two have been considered, where in addition the measurements can be split in two separate groups. In this case it turned out that the bounds were always reached with commuting observables. Our examples show that this is usually not the case, when longer measurement sequences are considered.

**Discussion and conclusions.**—For interpreting our results, let us note that our scenario is more general than the scenarios considered by Leggett and Garg and Kochen and Specker. Leggett and Garg consider a special time evolution $\varrho(t) = U(t)\varrho(0)U^\dagger(t)$, which is mapped in the Heisenberg picture onto the observables. In our case, \[54x70\] sources. We calculate the sequential bound for the case of violation with the use of postquantum no-signalling relations \[30\] and compute the corresponding Tsirelson-like inequality by Yu and Oh, as well as recent improvements \[30\]. For each inequality, the following numbers are given: the maximum value for noncontextual hidden variable (NCHV) models, the state-independent quantum violation in three-dimensional systems (obtained in Refs. \[28, 30\]), the algebraic maximum and the maximal value that can be attained in quantum mechanics for the sequential measurements. The latter bound is higher than the state-independent quantum value, since the observables do not have to obey the compatibility relations occurring in the Kochen-Specker theorem. Notice that the sequential bound is obtained as a maximization over the set of possible observables and states, thus it is in general state-dependent. Interestingly, in all cases the maximal quantum values are significantly below the algebraic maximum.

**TABLE I. Bounds on the quantum correlations for the Kochen-Specker inequalities in the most basic scenario.** Three inequalities were investigated: First, the original inequality proposed in Ref. \[28\] and the optimal inequalities from Ref. \[30\] with measurement sequences of length two (Opt2) and length three (Opt3). For each inequality, the following numbers are given: the maximum value for noncontextual hidden variable (NCHV) models, the state-independent quantum violation in three-dimensional systems (obtained in Refs. \[28, 30\]), the algebraic maximum and the maximal value that can be attained in quantum mechanics for the sequential measurements. The latter bound is higher than the state-independent quantum value, since the observables do not have to obey the compatibility relations occurring in the Kochen-Specker theorem. Notice that the sequential bound is obtained as a maximization over the set of possible observables and states, thus it is in general state-dependent. Interestingly, in all cases the maximal quantum values are significantly below the algebraic maximum.
the observables are not connected via unitaries; this corresponds to a more general time evolution. Compared with the Kochen-Specker scenario, our approach is more general since it does not assume that the measurements in a sequence are commuting. Nevertheless, if one wishes to connect existing noncontextuality inequalities to information processing tasks, it is important to know the maximal quantum values (also if the observables do not commute), in order to characterize the largest quantum advantage possible.

Furthermore, we emphasize that in our derivation it was assumed that the measurements are described by projective measurements and this condition is indeed important. In fact, this sheds light on the role of projective measurements: one can easily construct classical devices with a memory, which give for sequential measurements as in Eq. (2) the algebraic maximum $S_5 = 5$. These classical devices must also have a quantum mechanical description. Our results show, however, that in this quantum mechanical description more general than projective measurements must occur and a more general dynamical evolution than the projection is required. From this perspective, our results prove that the memory that can be encrypted in quantum systems by projective measurements is bounded.

Our results lead to the question of why quantum mechanics does not allow us to reach the algebraic maximum of temporal correlations, as long as projective measurements are considered. We believe that proper generalizations of concepts such as information causality and communication complexity might play a role here, but we leave this question for further research. A first step in explaining quantum mechanics from information theoretical principles lies in the precise characterization of all possible temporal quantum correlations, and our work presents an operational solution to this problem.

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A1: Discussion of the simplest Leggett-Garg scenario

In this part we provide some further details about how to determine the set of possible quantum values for the simplest non-trivial Leggett-Garg scenario as shown in Fig. 2 of the main text. Here it is assumed that one can measure an observable $M$ at three different time instances $t_1, t_2, t_3$ as shown in Fig. 1 of the main text, which gives rise to three different observables $A_i = M(t_i)$ with $i = 1, 2, 3$.

However, rather than being interested in determining the full sequential probability $P(r|s)$ for all possible combinations we are here only interested in some limited information, namely only for the correlation space. This means that from a general distribution we only want to reproduce the correlations terms $\langle A_i A_j \rangle_{\text{seq}}$ with $1 \leq i < j \leq 3$ each defined by

$$\langle A_i A_j \rangle_{\text{seq}} = P(r_i = r_j|i,j) - P(r_i \neq r_j|i,j).$$  \hspace{1cm} (14)

Thus we want to characterize the set

$$S_{\text{qum}} = \{q_{ij} \in \mathbb{R}^3 : q_{ij} = \langle A_i A_j \rangle_{\text{seq}}, \langle A_i A_j \rangle_{\text{seq}} \text{ has projective quantum rep.}\}.$$  \hspace{1cm} (15)

For this we refer to problem given by Eq. 4 of the main text, with

$$X = \begin{bmatrix} 1 & \langle A_1 A_2 \rangle_{\text{seq}} & \langle A_1 A_3 \rangle_{\text{seq}} \\ \langle A_1 A_2 \rangle_{\text{seq}} & 1 & \langle A_2 A_3 \rangle_{\text{seq}} \\ \langle A_1 A_3 \rangle_{\text{seq}} & \langle A_2 A_3 \rangle_{\text{seq}} & 1 \end{bmatrix}. \hspace{1cm} (16)$$

Any matrix of this form has a sequential projective quantum representation if and only if $X$ is positive semidefinite. However a matrix satisfies $X \geq 0$ if and only if the determinant of all principal minors are non-negative. This gives

$$S_{\text{qum}} = \{q_{ij} \in \mathbb{R}^3 : |q_{ij}| \leq 1, 1 + 2q_{12}q_{13}q_{23} \geq q_{12}^2 + q_{13}^2 + q_{23}^2\}. \hspace{1cm} (17)$$

which is the plotted region of Fig. 2 of the main text.

We mention that via the general method one can also in principle determine the achievable probability distribution of a general scenario. However, this requires the solution of a SDP with some unknown entries, and hence an analytic solution is in general not accessible.

A2: Detailed discussion of bounds for the $N$-cycle inequalities

We first need the general form [21] for Eq. (10) of the main text

$$S_N(\gamma) = \sum_{i=0}^{N-1} \gamma_i \langle A_i A_{i+1} \rangle_{\text{seq}}, \hspace{1cm} (18)$$

where the indices are taken modulo $N$ and $\gamma = (\gamma_0, \ldots, \gamma_{N-1}) \in \{-1, 1\}^N$ with an odd number of $-1$. Since any two assignments $\gamma$ and $\gamma'$ can be converted into each other via some substitutions $A_i \rightarrow -A_i$, the quantum bound does not depend on the particular choice of $\gamma$. For the case odd $N$, we can consider the expression

$$S_N = -\sum_{i=0}^{N-1} \langle A_i A_{i+1} \rangle_{\text{seq}}, \hspace{1cm} (19)$$
with index $i$ taken modulo $N$. The optimization problem in Eq. (4) of the main text, therefore, can be expressed as

$$\begin{align*}
\text{maximize:} & \quad \frac{1}{2} \text{Tr}(WX) \\
\text{subjected to:} & \quad X = X^T \succeq 0 \text{ and } X_{ii} = 1 \text{ for all } i, \quad (20)
\end{align*}$$

where $W$ is the circulant symmetric matrix

$$W = \begin{bmatrix}
0 & 1 & \ldots & 0 & 1 \\
1 & 0 & \ddots & \vdots & \vdots \\
\vdots & \ddots & \ddots & 1 & \vdots \\
0 & \ldots & \ldots & 0 & 1 \\
1 & 0 & \ldots & 1 & 0
\end{bmatrix}. \quad (21)$$

The condition $X \succeq 0$, i.e. $v^T X v \geq 0$ for any real vector $v$, follows from the fact that $(A_iA_j)_{seq} = \frac{1}{2} \text{Tr}[g(A_iA_j + A_jA_i)]$ and the fact that the matrix $Y = \text{Tr}[g(A_iA_j)]$ fulfills $v^T Y v \geq 0$ for any real vector $v$, and $X$ is the real part of $Y$.

By using the vector $\lambda = (\lambda_1, \ldots, \lambda_N)$, the dual problem for the semidefinite program in Eq. (20) can be written as (see Ref. [15] for a general treatment and Ref. [17] for the discussion of a similar problem)

$$\begin{align*}
\text{minimize:} & \quad \text{Tr}(\text{diag}(\lambda)) \\
\text{subjected to:} & \quad -\frac{1}{2} W + \text{diag}(\lambda) \succeq 0, \quad (22)
\end{align*}$$

where $\text{diag}(\lambda)$ denotes the diagonal matrix with entries $\lambda_1, \ldots, \lambda_N$.

Let us denote with $p$ and $d$ optimal values for, respectively, the primal problem in Eq. (20) and the dual problem in Eq. (22). Then $d \geq p$. We shall provide a feasible solution for the dual problem with $d = N \cos \left(\frac{\pi}{N}\right)$ and a feasible solution for the primal problem with $p = d$, this will guarantee the optimality of our primal solution.

We start by finding the maximum eigenvalue for $W$. Since $W$ is a circulant matrix, its eigenvalues can be written as $\mu_j = -2 \cos \left(\frac{2\pi j}{N}\right)$ for $j = 0, \ldots, N-1$, and $\mu_{\max} = 2 \cos \left(\frac{\pi}{N}\right)$ the maximum eigenvalue.

For a pair of Hermitian matrices $A, B$, it holds $\mu_{\min}(A + B) \geq \mu_{\min}(A) + \mu_{\min}(B)$, where $\mu_{\min}$ denotes the minimum eigenvalue. Therefore, $\lambda = (\cos \left(\frac{\pi}{N}\right), \ldots, \cos \left(\frac{\pi}{N}\right))$ is a feasible solution for the dual problem and $\text{Tr}[\text{diag}(\lambda)] = N \cos \left(\frac{\pi}{N}\right)$, and $p \leq N \cos \left(\frac{\pi}{N}\right)$.

Now consider the matrix $X'_{ij} = (x_i, x_j)$, with $x_1, \ldots, x_N$ unit vectors in a 2-dimensional space such that the angle between $x_i$ and $x_{i+1}$ is $\frac{N-1}{N} \pi$, and $(\cdot, \cdot)$ denoting the scalar product. Clearly, $X'$ is positive semidefinite. Since $X'_{i,i+1} = -\cos \left(\frac{i\pi}{N}\right)$, it follows that $p = d = N \cos \left(\frac{\pi}{N}\right)$ and the solution $X'$ is optimal.

In order to prove that $X'$ can be obtained as matrix of expectation values for sequential measurements, we define for a 3-dimensional unit vector $\vec{a}$ the observable $\sigma_a = \vec{a} \cdot \vec{x}$, where $\vec{x}$ denotes the vector of the Pauli matrices. Then, by Eq. (3) of the main text, $(\sigma_a \sigma_b)_{seq} = \vec{a} \cdot \vec{b}$, independently of the initial quantum state $\rho$. In fact, explicit observables reaching this bound have already been discussed in the literature [11, 19].

For the case $N$ even, we can consider the expression

$$S_N = \sum_{i=0}^{N-2} (A_iA_{i+1})_{seq} - (A_0A_{N-1})_{seq}, \quad (24)$$

and the maximization problem can be expressed as a SDP as in Eq. (24), with the proper choice of the matrix $W$. Such a SDP has been solved in Ref. [17]. The solution is analogous to the previous one: A set of observables, for a two-level system, saturating the bound, again, independently of the quantum state, is given by observables $A_i = \vec{a} \cdot \vec{x}_i$, where the vectors $x_i$ are on a plane with an angle $\frac{\pi}{N}$ separating $x_i$ and $x_{i+1}$.

As opposed to the $N$ odd case, such a bound can be also reached with commuting operators, this corresponds to the well known maximal violation of Braunstein-Caves inequalities [17].

The above results prove that the bound computed in Ref. [19] for sequential measurements on qubits, coinciding with the value explicitly obtained in Ref. [11], is valid for any dimension of the quantum system on which measurements are performed.

Finally, we stress that the construction of the above set of observables from the solution of the SDP, i.e., the matrix $X$ or the set of vectors $\{x_i\}$ such that $X_{ij} = (x_i, x_j)$, is general. We recall that the vectors $\{x_i\}$ can be obtained, e.g., as the columns of the matrix $\sqrt{X}$ and, therefore, the dimension of the subspace spanned by them is equal to the rank of the matrix $X$. In the previous case, since we were dealing with vectors in dimension $d \leq 3$, we used the property of Pauli matrices

$$\{\sigma_a, \sigma_b\} = \sigma_a \sigma_b + \sigma_b \sigma_a = 2(\vec{a} \cdot \vec{b}) \mathbb{1}. \quad (25)$$

For matrices $X$ with higher rank, the corresponding vectors $\{x_i\}$ will span a real vector space $V$ of dimension $d > 3$. Now for general complex vector spaces $V$ with a symmetric bilinear form $(,)$, an analogue of Eq. (25), namely

$$\{A_v, A_u\} = 2(v, u) \mathbb{1}, \quad \text{for any } u, v \in V \quad (26)$$

can be established by a representation of associated Clifford algebra, cf. Ref. [33, 34].

As a consequence, for every positive semidefinite real matrix $X$ with diagonal elements equal to 1, one can find...
a set of unit vectors \( \{ x_i \} \) giving \( X_{ij} = (x_i, x_j) \) and a set of \( \pm 1 \)-valued observables \( \{ A_i \} \), associated with \( \{ x_i \} \), such that

\[
\langle A_i A_j \rangle_{\text{seq}} = \text{Tr} \left[ \frac{1}{2} \rho (A_i A_j + A_j A_i) \right] = (x_i, x_j),
\]

(27)

for all quantum states \( \rho \). In particular, if the rank of \( X \) is \( d \), such operators can be chosen as \( 2^d \times 2^d \) Hermitian matrices [35]. This shows the completeness of the simplified method.

\[\text{A3: Completeness of the general method}\]

In this part we shortly comment on the completeness of the presented general method. As pointed out, this has already been proven indirectly in the context of the spatial bipartite case [23].

At first let us change slightly the notation in order to make it closer to the one used in Ref. [23]. In the following we do not explicitly consider the matrix \( M \) from the main text, but rather a slightly smaller matrix where one erases some trivial constraints. In the following the set \( \{ E_i \} \) contains all projectors \( \Pi_k \), but one of the outcomes \( k \) from each setting \( s \) is left out. We also use a single subscript to identify setting and outcome. Then the matrix

\[
\chi_{uv}^n = \text{Tr}[E(u)E(v)\rho]
\]

(28)

with \( u = (u_1, u_2, \ldots, u_l) \) is built from all products \( E(u) = E_{u_1}E_{u_2}\cdots E_{u_l} \) of the operators \( \{ E_i \} \) of at most length \( l \leq n \), and the single extra “sequence” \( u = 0 \) of the identity operator, \( E(0) = 1 \). Again this matrix has to satisfy linear relations parsed as \( \chi_{uv}^n = \chi_{u'v'}^n \), if the operators fulfill \( E(u)E(v)\dagger = E(u')E(v')\dagger \) as a consequence of the orthogonality properties of projectors, and that \( \chi^n \geq 0 \).

That this matrix is positive semidefinite can be verified as follows: Let us first assume that there exists a sequential projective quantum representation. Consider the operator \( C = \sum_n c_n E(u)\dagger \) with arbitrary \( c_n \in \mathbb{C} \) and evaluate the expectation value of \( CC\dagger \), which provides

\[
\text{Tr}(CC\dagger \rho) = \sum_{u,v} c_u \text{Tr}[E(u)\dagger E(v)\rho] c_v^* \quad (29)
\]

\[
= \sum_{u,v} c_u \chi_{uv}^n c_v^* \geq 0. \quad (30)
\]

The final inequality holds because \( CC\dagger \geq 0 \) and \( \rho \geq 0 \) are both positive semidefinite operators. Since \( c_n \in \mathbb{C} \) are arbitrary the condition given by Eq. (30) means that \( \chi^n \geq 0 \) is positive semidefinite.

For the reverse one needs a way to construct an explicit sequential projective quantum representation out of the matrix \( \chi^n \) satisfying the above properties. For this, clearly more difficult part, we refer to Ref. [23] and just mention the solution. For the given positive semidefinite matrix \( \chi^n \) one associates a set of vectors \( \{|e_n\} \) by the relation \( \chi_{uv}^n = \langle e_u | e_v \rangle \). From this set of vectors one now constructs an appropriate state and corresponding projective measurements by \( \mathcal{H} = \text{span}(\{|e_n\}) \), \( \hat{\rho} = |e_0\rangle\langle e_0| \), and \( \hat{E}_i = \text{proj}(\text{span}(\{|e_n| : u_i = i\})) \) where proj means the projector onto the given subspace. That these solutions satisfies all the required constraints is shown in the proof of Theorem 8 of Ref. [23]. An analogous mathematical result, valid only for the case of dichotomic observables, has been presented also in Ref. [25].

In the spatial case considered in Ref. [23], some of these operators, additionally, have to commute since they should correspond to measurements onto different local parts. This cannot be inferred, in general, by a finite level \( \chi^n \) and this is eventually the reason why in the spatial case arbitrary high order terms have to be considered. However, luckily, since in our situation the measurements of different settings may well fail to commute we can rely on a finite level \( n \).

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