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]

$$\mathcal{B} = \langle A_1 \otimes B_1\rangle + \langle A_1 \otimes B_2\rangle + \langle A_2 \otimes B_1\rangle - \langle A_2 \otimes B_2\rangle, \quad (1)$$

where A_i and B_j are measurements on two different particles. On the one hand, local realistic models obey the CHSH inequality $\mathcal{B} \leq 2$, which is violated in quantum mechanics. On the other hand, the maximal quantum value is upper bounded by $\mathcal{B} \leq 2\sqrt{2}$, 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 $\mathcal{B} = 4$ 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 violated [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

$$\mathcal{S}_5 = \langle A_1A_2\rangle_{\text{seq}} + \langle A_2A_3\rangle_{\text{seq}} + \langle A_3A_4\rangle_{\text{seq}} + \langle A_4A_5\rangle_{\text{seq}} - \langle A_5A_1\rangle_{\text{seq}} \quad (2)$$

has been considered [11,12]. Here, $\langle A_iA_j\rangle_{\text{seq}}$ 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 $\mathcal{S}_5 \leq 3$ 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

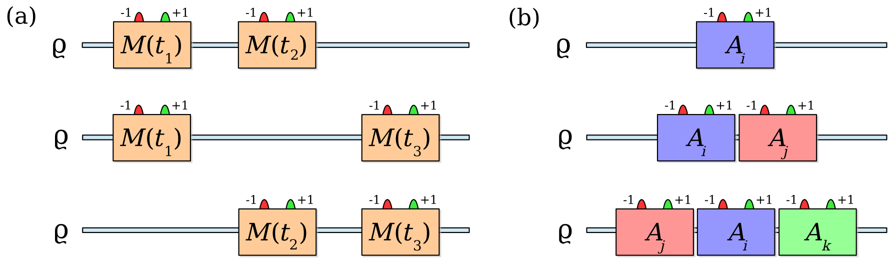

FIG. 1 (color online). Sequential measurements occur in two different scenarios. (a) In the Leggett-Garg scenario, one takes a single observable M that measures whether the physical system is in one of two possible macroscopic states. Then, one considers the correlations between these measurements at three different times, $\langle M(t_1)M(t_2)\rangle_{\rm seq}$, $\langle M(t_1)M(t_3)\rangle_{\rm seq}$, and $\langle M(t_2)M(t_3)\rangle_{\rm seq}$. The values predicted by quantum mechanics contradict the assumption that the physical system is in any of these macroscopic states at any time and that the measurement reveals this state without disturbing it. (b) In the Kochen-Specker scenario, one considers a set of observables A_i. Some of these observables are compatible and can therefore be measured simultaneously or in a sequence without any disturbance. Then one measures the correlations of simultaneous or sequential measurements of compatible observables, such as $\langle A_i\rangle_{\rm seq}$, $\langle A_iA_j\rangle_{\rm seq}$, and $\langle A_jA_iA_k\rangle_{\rm seq}$. For these correlations, one finds that quantum mechanics contradicts the assumption of noncontextuality. This assumption states that the result of a measurement should not depend on which other compatible observables are measured along with it. It should be noted, however, that the situation considered in this Letter is more general than case (a) or (b), since no assumption about the time evolution or the compatibility of observables is made.

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 ± 1 is described by two projectors Π_+ and Π_- 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., $\varrho \mapsto \Pi_\pm \varrho \Pi_\pm / \mathrm{Tr}(\varrho \Pi_\pm)$. Applying this scheme to the case of sequential measurements, one finds that the sequential mean value can be written as

$$\langle A_iA_j\rangle_{\rm seq} = \frac{1}{2}[\mathrm{Tr}(\varrho A_iA_j) + \mathrm{Tr}(\varrho A_jA_i)]. \tag{3}$$

It is interesting to notice that for pairs of ± 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 $\mathcal{S}_5$ in Eq. (2) can be determined. First, we consider a set $\mathcal{A} = \{A_i\}$ of ± 1-valued observables and a general expression $C = \sum_{ij}\lambda_{ij}\langle A_iA_j\rangle_{\rm seq}$. 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 $X_{ij} = \langle A_iA_j\rangle_{\rm seq}$. 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 $v^TXv \geq 0$ for any vector v), denoted as $X \succeq 0$ (see Supplemental Material [17]). A similar construction for the matrix X, together with the optimization problem below, has been considered before in relation with Bell inequalities [18]. 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

$$\begin{aligned} &\text{maximize: } \sum_{ij}\lambda_{ij}X_{ij}, \\ &\text{subjected to: } X = X^T \succeq 0 \text{ and for all } i,\ X_{ii} = 1. \end{aligned} \tag{4}$$

Since all matrices X that can originate from a sequences 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 $\mathcal{S}_5$. 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 [19]. In the case of $\mathcal{S}_5$, this optimization can even be solved analytically and gives

$$\mathcal{S}_5 \leq \frac{5}{4}(1+\sqrt{5}) \approx 4.04. \tag{5}$$

It turns out that appropriately chosen measurements on a qubit already reach this value (see Supplemental Material [17] and Refs. [11,20]). 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 Supplemental Material [17]). Finally, note that if the observables in each sequence are required to commute, then the maximal quantum value for $\mathcal{S}_5$ is known to be $\Omega_{\rm QM} = 4\sqrt{5} - 5 \approx 3.94$ [21,22].

The general method.—The above method can only be used for correlations terms of sequences of at most two ± 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 $\mathbf{r} = (r_1, r_2, \ldots, r_n)$ the results of an n-length sequence obtained by using the setting $\mathbf{s} = (s_1, s_2, \ldots, s_n)$. 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

$$P(\mathbf{r}|\mathbf{s}) \equiv P_{\text{seq}}(r_1, r_2, \ldots, r_n|s_1, s_2, \ldots, s_n). \quad (6)$$

In the case of projective quantum measurements, each individual result r of any setting s is associated with a projector Π_r^s, which altogether satisfy two requirements: for each setting the operators must sum up to the identity, i.e., $\sum_r \Pi_r^s = \mathbb{1}$ and they satisfy the orthogonality relations $\Pi_r^s \Pi_{r'}^s = \delta_{rr'} \Pi_r^s$, where $\delta_{rr'}$ is the Kronecker symbol. Finally, after the measurement with setting s and result r, the quantum state is transformed according to the rule $\varrho \mapsto \Pi_r^s \varrho \Pi_r^s / P(r|s)$.

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

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

with the shorthand $\Pi(\mathbf{r}|\mathbf{s}) = \Pi_{r_1}^{s_1}\Pi_{r_2}^{s_2}\cdots\Pi_{r_n}^{s_n}$.

Whether a given distribution $P(\mathbf{r}|\mathbf{s})$ indeed has such a representation can be answered via a so-called matrix of moments, which often appears in moment problems [18,23–25]. This matrix, denoted as M in the following, contains the expectation value of the products of the above-used operators $\Pi(\mathbf{r}|\mathbf{s})$ at the respective position in the matrix. In order to identify this position, we use as a label the abstract operator sequence $\mathbf{r}|\mathbf{s}$ for both row and column index. In this way the matrix is defined as

$$M_{\mathbf{r}|\mathbf{s};\mathbf{r}'|\mathbf{s}'} = \langle \Pi(\mathbf{r}|\mathbf{s})\Pi(\mathbf{r}'|\mathbf{s}')^\dagger \rangle. \quad (8)$$

Whenever this matrix is indeed given by a sequential projective quantum representation, the matrix M satisfies two conditions: (a) linear relations of the form $M_{\mathbf{r}|\mathbf{s};\mathbf{k}|\mathbf{l}} = M_{\mathbf{r}'|\mathbf{s}';\mathbf{k}'|\mathbf{l}'}$ if the underlying operators are equal as a consequence of the properties of normalization and orthogonality of projectors; (b) $M \succeq 0$ since $v^\dagger M v \geq 0$ holds for any vector v, because such a product can be written as the expectation value $\langle CC^\dagger \rangle_\varrho \geq 0$ 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 $M_{\mathbf{r}|\mathbf{s};\mathbf{r}|\mathbf{s}} = P(\mathbf{r}|\mathbf{s})$. The main point, however, is the converse statement: given a moment matrix with properties (a) and (b) above, the associated probability distribution $P(\mathbf{r}|\mathbf{s})$ always has a sequential projective quantum representation (see Supplemental Material [17]).

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 [23,24], 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 [24], and an analogous mathematical result, valid for the special case of dichotomic observables, has been presented in Ref. [26] in the context of polynomial optimization problems (see Supplemental Material [17]).

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

$$\mathcal{S} = \langle M(t_1)M(t_2)\rangle_{\text{seq}} + \langle M(t_2)M(t_3)\rangle_{\text{seq}} - \langle M(t_1)M(t_3)\rangle_{\text{seq}} \leq 1. \quad (9)$$

This bound holds for macrorealistic models, and it has been shown that in quantum mechanics values up to $\mathcal{S} = 3/2$ can be observed [10,11,13]. Our methods not only allow us 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 Supplemental Material [17].

Second, we consider generalizations of the Eq. (2) with a larger number of measurements, known as N-cycle inequality [21,22],

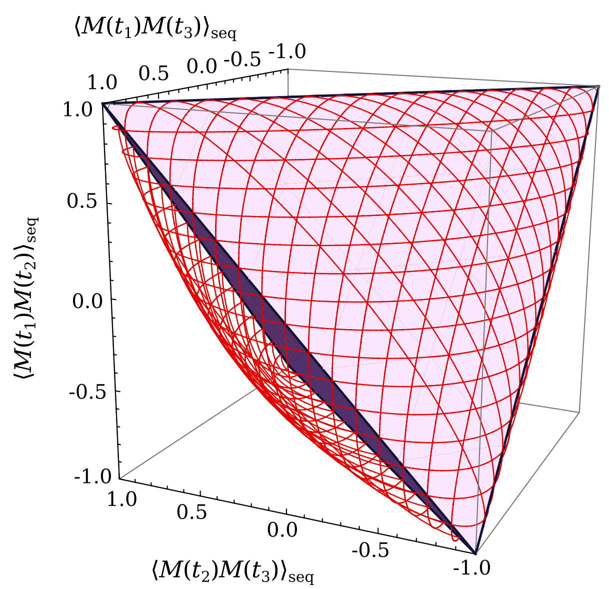

FIG. 2 (color online). Complete characterization of the possible quantum values for the simplest Leggett-Garg scenario. In this case, three different times are considered, resulting in three possible correlations $\langle M(t_1)M(t_2)\rangle_{\text{seq}}$, $\langle M(t_1)M(t_3)\rangle_{\text{seq}}$, and $\langle M(t_2)M(t_3)\rangle_{\text{seq}}$. In this three-dimensional space, the possible classical values form a tetrahedron, characterized by Eq. (9) and variants thereof. The possible quantum mechanical values form a strictly larger set with curved boundaries.

$$\mathcal{S}_N = \sum_{i=0}^{N-2} \langle A_i A_{i+1} \rangle_{\text{seq}} - \langle A_{N-1} A_0 \rangle_{\text{seq}}. \qquad (10)$$

For this case, everything can be solved analytically (see Supplemental Material [17]) leading to the bound

$$\mathcal{S}_N \le N \cos\left(\frac{\pi}{N}\right), \qquad (11)$$

which can be reached by suitably chosen measurements. This value has already occurred in the literature [11,20], 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 [20], and also for Bell inequalities this has been observed [27,28].

As a third application, we consider the noncontextuality scenario recently discovered by S. Yu and C. H. Oh [29]. 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 [30], 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 [31] and compute the corresponding Tsirelson-like bounds. We emphasize that our results are not directly related to the phenomenon of quantum contextuality, since no compatibility of the measurements is assumed, but the results 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 I.

Another class of inequalities is given by the guess-your-neighbor's-input inequalities [32], which if viewed as multipartite inequalities, show no quantum violation but a violation with the use of postquantum no-signaling resources. We calculate the sequential bound for the case of measurement sequences of length three, instead of measurement on three parties. We consider

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

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

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

while it is known that $\Omega_{C,Q} = 1$ and $\Omega_{NS} = 4/3$, where the indices C, Q, S, NS label, respectively, the classical, quantum, sequential and no-signaling 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.

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. [29] and the optimal inequalities from Ref. [31] 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. [29,31] for joint measurements of compatible observables), 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.

Inequality	NCHV bound	State-independent quantum value	Algebraic maximum	Sequential bound
Yu-Oh	16	$50/3 \approx 16.67$	50	17.794
Opt2	16	$52/3 \approx 17.33$	52	20.287
Opt3	25	$83/3 \approx 27.67$	65	32.791

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, 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 $\mathcal{S}_5 = 5$. 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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