Unified approach to contextuality, non-locality, and temporal correlations

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We highlight the existence of a joint probability distribution as the common underpinning assumption behind Bell-type, contextuality, and Leggett-Garg-type tests. We then present a procedure to translate contextual scenarios into temporal Leggett-Garg-type and spatial Bell-type ones. To demonstrate the generality of this approach we construct a family of spatial Bell-type inequalities. We show that in Leggett-Garg scenario a necessary condition for contextuality in time is given by a violation of consistency conditions in Consistent Histories approach to quantum mechanics.

I. INTRODUCTION

Classical physical theories such as general relativity, electrodynamics and thermodynamics describe a universe where acts of observation merely reveal underlying reality. For instance, an electromagnetic field or a black hole exists objectively at all times independently of whether we choose to observe it or not. Quantum theory of matter is different. It was theoretically demonstrated by Bell in 1964 [1] and by Kochen and Specker (KS) in 1967 [2] that quantum mechanical predictions depend on the act of observation. Both of these predictions found confirmation in experiments: Bell inequalities were violated in numerous laboratories [3–7] as were certain inequalities encapsulating KS ideas [8, 9]. In 1985 Leggett and Garg (LG) presented a related notion of macroscopic realism [10] asserting that a macroscopic system should at all times be in one of its macroscopically distinguishable states that do not change if a measurement is performed on the system.

Although the theorems by Bell, KS and LG seem different they are in fact based on the same underlying hypothesis. They all contrast quantum mechanical predictions with predictions of theories that assume the existence of a joint probability distribution for the outcomes of all possible measurements one can perform on a physical system. More precisely, consider measurements from the set $S = \{X_1, X_2, \ldots, X_N\}$, such that measurement $X_j$ yields an outcomes $x_j$, with $j = 1, 2, \ldots, N$. For some of these measurements a joint probability distribution, of the type $p_{\text{exp}}(x_i, x_j)$, can be experimentally obtained while for other subsets such experimental joint probability distributions cannot be measured. For example, according to quantum theory it is impossible to construct a device capable of simultaneously measuring two non-commuting observables on a single system. Objective reality assumes that nevertheless there exists a joint probability distribution for the full set of these observables, $p(x_1, x_2, \ldots, x_N)$. Depending on a physical scenario considered, the lack of such joint probability is called quantum non-locality, contextuality or violation of macroscopic realism.

In Bell-type experiments the set $S$ is divided into two or more groups of measurements $S = A \cup B \cup \ldots$, such that each group represents a set of measurements performed by spatially separated observers. If one arranges a situation in which the measurements are space-like separated, special relativity dictates a natural assumption that the outcomes obtained on individual systems do not depend on the parameters in distant laboratories. In such a case the existence of the joint probability distribution is known as the assumption of local realism [11], first formulated in 1935 in the important paper by Einstein, Podolsky and Rosen [12]. The fact that quantum mechanical predictions cannot be described in this way is sometimes phrased as quantum non-locality.

In KS-type experiments there are no spatially separated systems. For instance, the simplest KS scenario introduced by Klyachko et. al. [13] contains a set of five measurements for which one can experimentally establish joint probabilities $p_{\text{exp}}(x_1, x_2), p_{\text{exp}}(x_2, x_3), \ldots, p_{\text{exp}}(x_5, x_1)$. If the joint probability distribution for the outcomes of all these observables exists, $p(x_1, x_2, \ldots, x_5)$, such a model is known as a non-contextual realistic theory. In this sense, each Bell-type experiment is a special case of KS experiment where the context of measurements is provided by spatial separation of observers.

LG-type scenarios are similar to the KS-type experiments in that a single physical system is being interrogated. In the LG setting there is a single physical property $X_t$ that evolves in time. This property is measured at different times $t_1, t_2, \ldots$ and probabilities $p_{\text{exp}}(x_{t_1}, x_{t_2})$ are estimated for suitable time slices. The existence of the joint probability distribution for the outcomes at all times, $p(x_{t_1}, x_{t_2}, \ldots)$, whose marginals agree with $p_{\text{exp}}(x_{t_1}, x_{t_j})$, is known as the assumption of macroscopic realism. In quantum mechanics the lack of this joint probability distribution is due to intermediate quantum evolution and the invasive nature of quantum measurements.
Since all these cases share the same mathematical background one expects to find correspondence between them. Here we reveal this correspondence and use it to derive new inequalities. First we review a simple test of contextuality of a single system and then explain how it can be extended to both a temporal scenario and a spatial scenario on two subsystems. Next, we discuss how to translate between general correlations of two measurements realised in three different scenarios: contextual, non-local and temporal. We conclude with observations relating our correspondence to consistent histories and quantum cryptography.

II. COMPATIBLE MEASUREMENTS ON A SINGLE SYSTEM

We first study the scheme proposed by Klyachko-Can-Biniogi-Can-Can (KCBS) [13]. Consider five dichotomic ±1 measurements $X_j$ on a single system where each $X_j$ is compatible with $X_{j-1}$ and $X_{j+1}$ for $j = 0, \ldots, 4$, and sums are modulo 5. Compatible, here, means from the operational point of view that these observables can be measured jointly or sequentially, with an assumption that sequential measurements do not affect each other. More precisely, if $X_j$ is measured first, then the measurement of $X_i$ does not change the outcome of $X_j$, which can be confirmed by a subsequent measurement of $X_j$, i.e., the measurement sequence is $X_j \rightarrow X_i \rightarrow X_j$. This property guarantees non-invasiveness of measurements.

The possibility of joint probability distribution of the outcomes of all physical observables on a single system can be tested by the following KCBS inequality proposed by Ref. [13]:

\[ \sum_{j=0}^{4} \langle X_j X_{j+1} \rangle \geq -3. \] (1)

For completeness we present a proof of this inequality. By definition each correlation function is given by

\[ \langle X_i X_j \rangle = \sum_{x_i, x_j = \pm 1} x_i x_j p(x_i, x_j). \] (2)

By assumption there exists a joint probability distribution for all variables $X_i$, e.g.:\n
\[ \langle X_0 X_1 \rangle = \sum_{x_0, \ldots, x_4 = \pm 1} x_0 x_1 p(x_0, x_1, x_2, x_3, x_4). \] (3)

Note that for a non-contextual assignment of values $x_j = \pm 1$ we have $\sum_{j=0}^{4} x_j x_{j+1} \geq -3$, which can be directly verified. Combining all above expressions we get:

\[ \langle X_0 X_1 \rangle + \langle X_1 X_2 \rangle + \langle X_2 X_3 \rangle + \langle X_3 X_4 \rangle + \langle X_4 X_0 \rangle = \sum_{x_0, \ldots, x_4 = \pm 1} p(x_0, x_1, x_2, x_3, x_4) \sum_{j=0}^{4} x_j x_{j+1} \geq \sum_{x_0, \ldots, x_4 = \pm 1} p(x_0, x_1, x_2, x_3, x_4) (-3) = -3. \]

By definition we have $X_0 X_1 = 0$. Maximal quantum violation of the above inequality (so-called Tsirelson bound) within this framework is known to be [14, 15]:

\[ T_{\text{context}} = 5 - 4\sqrt{5} \approx -3.94. \] (4)

III. TEMPORAL KCBS INEQUALITY

In quantum mechanics the compatibility is provided by $[X_j, X_{j\pm 1}] = 0$. Maximal quantum violation of the above inequality (so-called Tsirelson bound) within this framework is known to be [14, 15]:

\[ T_{\text{context}} = 5 - 4\sqrt{5} \approx -3.94. \] (4)

Instead of studying contextuality using the KCBS inequality we investigate a temporal-non-contextual-inequality whose construction roughly parallels seminal work done by Leggett and Garg [12] and continued in [16, 17].

Consider a dichotomic ±1 measurement, $X_t$, which is conducted at time $t = \{t_0, t_1, \ldots, t_4\}$. If we make successive measurements at two sequential times, then we can construct two point temporal correlations $\langle X_{t_0} X_{t_1} \rangle$, $\langle X_{t_1} X_{t_2} \rangle$, $\langle X_{t_2} X_{t_3} \rangle$, $\langle X_{t_3} X_{t_4} \rangle$. These two-point temporal correlations naturally lead to a temporal analogue of the KCBS inequality

\[ \langle X_{t_0} X_{t_1} \rangle + \langle X_{t_1} X_{t_2} \rangle + \langle X_{t_2} X_{t_3} \rangle + \langle X_{t_3} X_{t_4} \rangle \geq -3. \] (5)

This inequality will be satisfied whenever there is a joint probability distribution which ascribes predetermined outcomes to the measurements $X_t$ at all times $t_0, \ldots, t_4$.

The existence of the joint probability distribution in this scenario is tantamount to Leggett and Garg’s “macrorealism” condition [10]. Conversely, violation of the inequality (5) can be called contextuality in time.

In quantum mechanics the inequality (5) can be violated using a single spin-$\frac{1}{2}$ particle. We stipulate that in each run of the experiment we make precisely two measurements corresponding to a pair of observables $X_{t_i}$ and $X_{t_{i\pm 1}}$ for definitiveness, we specify the observable $X_{t_i}$ to be represented by a $\sigma_z$ Pauli operator measured at one of five distinct times, $t \in \{t_0, \ldots, t_4\}$. We initialise the spin in a completely mixed state and allow it to evolve under the unitary operator

\[ U = e^{i \frac{\pi}{8} \sigma_z}. \] (6)

For this scenario, the left-hand side of the inequality (5) attains the minimal value of $-4.045$ if we choose the time instances $t \in \{t_0, \ldots, t_4\} = \{0, 1, 2, 3, 4\}$. It has recently been proved by Gühne et. al. [13] that this is the maximum possible violation of inequality (5) by a qubit when pairs of sequential measurements do not commute. In order to calculate temporal correlations of ±1 measurements we use the following formula

\[ \langle X_{t_i} X_{t_{i+1}} \rangle = p_{i+1} q_{i+1} + p_{i-1} q_{i-1} - p_{i+1} q_{i-1} - p_{i} q_{i+1}, \] (7)

where $p_k$ denotes probability of outcome $k$ in the first measurement (at instant $t_1$), and $q_{ilk}$ denotes probability
of the outcome $l$ in the second measurement (at $t_2$) on condition that outcome $k$ occurred in the first one. In quantum mechanics, this formula reduces to

$$\langle X_{t_1}X_{t_2} \rangle = \frac{1}{2} \text{Tr} (\rho \{X_{t_1},X_{t_2}\}),$$

where $\{X_{t_1},X_{t_2}\}$ denotes the anti-commutator.

IV. NEW SPATIAL INEQUALITY AND ITS QUANTUM VIOLATION

Finally, the inequality (5) can be transformed into a Bell-type inequality testing the existence of a joint probability distribution for spatially separated local measurements. Within this framework $\langle X_iX_j \rangle = \langle A_iB_j \rangle$ are correlations obtained on space-like separated systems $A$ and $B$. The inequality (5) takes the form:

$$\langle A_0B_1 \rangle + \langle A_1B_2 \rangle + \langle A_2B_3 \rangle + \langle A_3B_4 \rangle + \langle A_4B_0 \rangle \geq -3$$

with additional constraint

$$\langle A_iB_i \rangle = 1 \quad \text{for all } i,$$

which means that $A_i$ and $B_i$ always have the same outcomes.

The inequality (9) together with the assumption $\langle A_1B_1 \rangle = 1$ resembles the original Bell scenario for three ±1 qubit measurements $A$, $B$, and $C$:\

$$1 + \langle B \otimes C \rangle \geq |\langle A \otimes B \rangle + \langle A \otimes C \rangle|,$$

where it was assumed that $\langle B \otimes B \rangle = -1$ due to correlations of the singlet state. The additional assumption of the outcome correlation of pairs of spatially separated measurements is often considered as a weakness of this type of nonlocality tests. In real experimental scenarios, other tests that do not require this assumption are preferred. Nevertheless, the inequality (9) can be used as a theoretical tool to refute local realistic description of quantum measurements and, what is more important, to establish a unified framework to describe noncontextuality, nonlocality and contextuality in time as different physical manifestations of the violation of the same mathematical property.

The optimal violation of (9) can be obtained for the state $\rho' = |\phi_+\rangle\langle\phi_+|$, with $|\phi_+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, and for measurements $A_i = \sigma_i \otimes 1$, $B_i = 1 \otimes \sigma_i$, where $i = 0, \ldots, 4$ and $\sigma_i = e^{i\frac{\pi}{4}} \sigma_x e^{-i\frac{\pi}{4}} \sigma_x$. Note that the state $|\phi_+\rangle$ has the property that for the qubit measurements in the $xz$-plane, $M(\alpha) = \cos \alpha \sigma_x + \sin \alpha \sigma_z$, one has $\langle \phi_+ | M(\alpha) \otimes M(\alpha) | \phi_+ \rangle = 1$. Therefore, the assumption $\langle A_iB_i \rangle = 1$ is fulfilled by this state.

On the level of quantum mechanics, the link between temporal and spatial correlations was noticed before [18]. This is a direct consequence of an extension of Tsirelson’s theorem on different representations of correlation matrices for quantum observables [19]. It says that the following two statements are equivalent:

1. There exists a Hilbert space $H$ together with Hermitian operators $A_1, \ldots, A_m, B_1, \ldots, B_n \in \mathcal{B}(H)$ fulfilling $A_i^2 = 1$, $B_i^2 = 1$, and a density matrix $\rho$ such that:

$$\langle A_kB_l \rangle = \frac{1}{2} \text{Tr} (\rho \{A_k,B_l\}).$$

2. There exist Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ together with Hermitian operators $A_1, \ldots, A_m \in \mathcal{B}(\mathcal{H}_A)$, $B_1, \ldots, B_n \in \mathcal{B}(\mathcal{H}_B)$ fulfilling $A_i^2 = 1$, $B_i^2 = 1$, and a density matrix $\rho'$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ such that:

$$\langle A_kB_l \rangle = \text{Tr} (\rho' \{A_k \otimes B_l\}).$$

What is very important and omitted in [18] is that the state $\rho'$, due to Tsirelson’s construction, has a very specific form. Namely, it has to fulfil the following relations:

$$\langle A_iB_j \rangle = \text{Tr} (\rho' A_i \otimes B_j) = 1, \quad \text{for } i = 1, \ldots, \min(m,n).$$

Equivalence between the two above statements implies that the Tsirelson bound of the Bell-type inequality (9) is the same as for the temporal inequality (9).

V. GENERALIZATION TO ARBITRARY NUMBER OF MEASUREMENTS

The approach to the KCBS scenario discussed above can be generalised in a straightforward manner to any test of contextuality that utilises two-point correlations. Up to now we discussed scenarios involving five measurements. In general, if one can experimentally evaluate $p_{\text{exp}}(x_i, x_{i+1})$ for $N$ dichotomic ±1 measurements $i = 0, \ldots, N-1$, the existence of joint probability distribution $p(x_0, \ldots, x_{N-1})$ implies that the following inequality is satisfied [18] [20]:

$$\sum_{i=0}^{N-2} \langle X_iX_{i+1} \rangle + (-1)^{N-1} \langle X_{N-1}X_0 \rangle \geq -N + 2.$$  (14)

Using our framework this inequality can be tested in three physical settings.

The first one is the contextuality test on a single system where co-measurability is provided by compatibility of measurements, i.e. there exists a device for which the outcomes of both measurements are always independent of the order in which they are performed.

In the second, temporal, setting one can treat the two-point correlations entering (14) as expectation values of two measurements performed at different times. The measurements here are no longer required to be compatible and the co-measurability is provided by temporal separation.

The implementation of the third, spatial, scenario depends on the parity of $N$. If $N$ is an even number there
exist a natural bipartition of measurements, \(X_{2i} = A_i\) and \(X_{2i+1} = B_i\), and the inequality is transformed to:

\[
\langle A_0B_0 \rangle + \langle A_1B_0 \rangle + \langle A_1B_1 \rangle + \ldots + \langle A_{(N-2)/2}B_{(N-2)/2} \rangle 
- \langle A_0B_{(N-2)/2} \rangle \geq -N + 2. \quad (15)
\]

However, in the case of odd \(N\), such bipartition does not exist and to bypass this problem we propose to double the number of measurements, i.e., Alice (Bob) has \(N\) measurements \(A_0, \ldots, A_{N-1}\) \((B_0, \ldots, B_{N-1})\). In addition we require perfect correlations between the corresponding local measurements, i.e., \(\langle A_iB_i \rangle = 1\) for all \(i\). This implies that the outcome of observable \(A_i\) and \(B_i\) is always the same. Consider now the following inequality

\[
\sum_{i=0}^{N-2} \langle A_iB_{i+1} \rangle + (-1)^{N-1} \langle A_{N-1}B_0 \rangle \geq -N + 2. \quad (16)
\]

The local realistic bound of \(-N + 2\) follows from the fact that although \(\langle A_iA_{i+1} \rangle\) is not directly measurable, due to our assumptions \(\langle A_iA_{i+1} \rangle = \langle A_iB_{i+1} \rangle\) and one can rewrite this spatial inequality using only the measurements of Alice in which the inequality has the form of (14).

The Bell inequalities (15) and (16) are violated by any \((e_1, e_2, \ldots, e_N)\) and \((f_1, f_2, \ldots, f_N)\).

VI. CONSISTENT HISTORIES APPROACH TO TEMPORAL INEQUALITIES

The violation of local realism and non-contextuality is a result of non-classical correlations between subsystems or between local observables. In quantum theory these correlations stem from entanglement or from commutation properties of local operators that are used to test non-contextuality. On the other hand, non-classical temporal correlations result from the lack of commutativity between the observables (in Heisenberg picture) that are sequentially measured. We now show that these correlations can be also interpreted as resulting from inconsistency of histories describing the measurement scenario. This is done within the Consistent Histories approach to quantum theory [21, 22]. The result might be anticipated as satisfying the consistency conditions allows ordinary probabilistic reasoning [21, 22] and guarantees non-invasiveness of intermediate measurements [23]. Nevertheless, it is instructive to see how the consistency condition naturally emerges in the context of temporal inequalities.

Consider two sequences of events \((e_1, e_2, \ldots, e_N)\) and \((f_1, f_2, \ldots, f_N)\). We assume that these events are ordered in time, i.e., \(e_i\) happens before \(e_j\) if \(i < j\) (similar for \(f_i\)). We refer to these sets as ‘history \(e\)’ and ‘history \(f\)’. In quantum theory these events correspond to projectors \(P_N^e, P_{N-1}^e, \ldots, P_N^f, P_{N-1}^f, \ldots, P_1^f\).

Next, consider operators \(C_e = P_N^e \ldots P_2^e P_1^e\) and \(C_f = P_N^f \ldots P_2^f P_1^f\). It is said that the two histories measured on a state \(\rho\) are consistent if and only if [22]:

\[
\text{Re} \left( \text{Tr} \left( C_e \rho C_f^\dagger \right) \right) = 0. \quad (18)
\]

This condition assures validity of ordinary probabilistic reasoning about joint events without going to any contradictions.

Next, consider the LG inequality in the form

\[
\langle X_1X_2 \rangle + \langle X_2X_3 \rangle + \langle X_1X_3 \rangle \geq -1, \quad (19)
\]

where \(X_i\) (\(i = 1, 2, 3\)) are \pm 1 observables. We associate the corresponding measurement events with projectors \(P_k^i\), where \(k = \pm 1\). Let us define a probability distribution for all three measurement outcomes \(p(X_1 = k, X_2 = l, X_3 = m) \equiv p(k, l, m)\) as

\[
p(k, l, m) = \text{Tr} \left( P_m^3 P_l^2 P_k^1 \rho P_k^1 P_l^2 P_m^3 \right), \quad (20)
\]

where the last term \(P_m^3\) is not necessary, but we put it for convenience. Note, that this probability distribution does not necessarily reproduce marginal probabilities, therefore it may not be a joint probability distribution that guarantees a classical model. It rather provides us with a link to the consistent histories formalism, where \(p(k, l, m)\) are probabilities of histories \((k, l, m)\). Each quantum correlation function entering (19) can be expressed in anal-
ogy to
\[
\langle X_2X_3 \rangle = \sum_k (p(\ast, k, k) - p(\ast, k, -k)),
\]
where, e.g., \( p(\ast, k, k) = \text{Tr}(P_k^{(3)} P_k^{(2)} P_k^{(1)}) \) is calculated by considering a hypothetical measurement at time \( t_1 \), and using \( \sum_k P_k^{(1)} = I \):
\[
p(\ast, k, k) = p(\ast, k, k) + p(-, k, k) + I(\ast, k, k),
\]
where we introduced the interference term \( I(\ast, k, k) = 2\text{Re} \left( \text{Tr} \left( P_k^{(3)} P_k^{(2)} P_k^{(1)} P_k^{(2)} P_k^{(3)} \right) \right) \). We therefore arrive at the following form of inequality \[19\]:
\[
\sum_k (4p(k, k) + I(\ast, k, k) + I(k, \ast, k)) - I(\ast, k, -k) - I(k, \ast, -k) \geq 0,
\]
where we also used the fact that \( I(k, \ast, \ast) = I(k, -k, \ast) = 0 \). A necessary condition for the violation of the inequality \[23\] is that at least one of the terms \( I(\ast, k, k), I(k, \ast, k), I(\ast, k, -k), I(k, \ast, -k) \) is nonzero. This however implies that at least one pair of the histories:
\[
\{(\ast, k, k), (-, k, k)\}, \{(k, \ast, k), (k, -k, k)\}
\]
\[
\{(\ast, k, -k), (-, k, -k)\}, \{(k, \ast, -k), (k, -k, -k)\}.
\]
contains inconsistent ones, which follows directly from \[18\].

A direct validation of this statement that does not utilise inequalities comes from noticing that \( p(k, l, m) \) provides a valid marginal probability in \[22\] only if \( I(\ast, k, k) = 0 \), ergo the histories \( (+, k, k) \) and \( (-, k, k) \) are consistent.

It is worth mentioning that the vanishing interference terms \( I(k, k, \ast) \) and \( I(k, -k, \ast) \) are related to the term \( \langle X_1X_2 \rangle \). Therefore only the terms \( \langle X_1X_3 \rangle \) and \( \langle X_2X_3 \rangle \) directly give rise to the quantum violation of the LG inequality \[19\] (Fig. 1).

Intuitively, the consistency conditions assure that the additivity of probabilities of single events is compatible with additivity of squared quantum probability amplitudes \[22\]. On the contrary, violation of these conditions implies that some interference terms between the probability amplitudes arise.

\[\text{VII. CONCLUSIONS}\]

We discussed Bell, Kochen-Specker, and Leggett-Garg experiments and showed that they are all different physical manifestations of the violation of the same underlying mathematical property — the existence of a joint probability distribution for all possible measurements that can be performed on the system. We introduced correspondence between these scenarios.

Note that this correspondence can be used to establish a link between the two acclaimed quantum key distribution protocols, the BB84 \[24\] protocol and the Ekert protocol \[25\]. Although the security of both protocols relies on different fundamental physical principles, mathematically speaking their security stems from the lack of a joint probability distribution. The Ekert protocol utilises quantum non-locality whereas BB84 relies on invasiveness of quantum measurements, effectively contradicting the assumptions of the macro-realism.

Utilizing the Consistent Histories approach to sequential measurements we found, that a necessary condition for violation of temporal Bell inequalities is existence of interference effects between probability amplitudes related to sequences of events.

We are confident this general framework will find further applications. For instance, one can easily approach the problem of mixed space and time quantum correlations \[26\] and has an attractive feature that it can be implemented numerically using standard modules for linear programming.

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During the completion of this work two independent papers covering similar topics appeared \[13\] \[26\].
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