Temporal Quantum Correlations and Leggett-Garg Inequalities in Multilevel Systems

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We show that the quantum bound for temporal correlations in a Leggett-Garg test, analogous to the Tsirelson bound for spatial correlations in a Bell test, strongly depends on the number of levels N that can be accessed by the measurement apparatus via projective measurements. We provide exact bounds for small N that exceed the known bound for the Leggett-Garg inequality, and we show that in the limit $N \to \infty$ the Leggett-Garg inequality can be violated up to its algebraic maximum.

Introduction.—Bell inequalities place fundamental bounds on the nature of correlations between spatially separated entities within a local hidden variable framework [1]. Leggett and Garg showed that *temporal* correlations obey similar inequalities based on assumptions of macroscopic realism and noninvasive measurability [2]. Quantum particles are bound neither by local hidden variables nor macroscopic realism and so can violate both Bell and Leggett-Garg inequalities (LGIs).

The maximum degree to which a quantum system can violate a Bell inequality is known as the Tsirelson bound [3], significantly less than the largest-conceivable value, the algebraic bound [4]. Violations of a Bell inequality beyond the Tsirelson bound would be evidence of new physics beyond quantum theory [6].

With interest in the LGIs growing (see Ref. [7] for a review), we ask here whether there is such a thing as a temporal Tsirelson bound for the LGIs. In the light of some recent results [8,9] and given the formal symmetry between the two types of inequality [10,11] and the general trend towards unification between temporal and spatial correlations [12–15], one would expect that the Tsirelson bound for the LGIs holds analogously to the spatial case. Surprisingly, and as we show here, this is not the case. By considering a broader class of projective measurements than hitherto considered, we show that the maximum quantum violation of the LGIs can exceed the Tsirelson value and that it increases with increasing system size, even up to the algebraic bound in the asymptotic limit.

Let us now be more concrete and consider the simplest LGI which, for dichotomous observable $Q = \pm 1$, reads

$$K_3 \equiv C_{21} + C_{32} - C_{31} \leq 1, \tag{1}$$

where $C_{\beta\alpha} = \langle Q(t_\beta)Q(t_\alpha) \rangle$ is the correlation function of variable Q at the two times $t_\beta \geq t_\alpha$. For a two-level system, the maximum quantum value of K_3 is $K_3^{\max} = \frac{3}{2}$ [2], which we shall refer to as the Lüders bound, $K_3^{\text{Lüders}} = \frac{3}{2}$, for reasons that will become clear shortly. It has been proven

rigorously that for measurements given by just two projectors, Π_+ and Π_-, onto eigenspaces associated with results $Q = +1$ and $Q = -1$, the maximum quantum value of K_3 is the same as for the qubit, *irrespective of system size* [9]. This has been reflected in several studies: The experiment of Ref. [16] on a three-level system obtained a maximum value of less than $3/2$; on the theory side, multilevel quantum systems such as a large spin [17], optoelectromechanical systems [18], and photosynthetic complexes [19] have also been observed to obey $K_3 \leq K_3^{\text{Lüders}}$. From this, one might conclude that nothing new is to be gained from considering higher-dimensional systems. Were this the case, the bound for the qubit would apply in all generality and $K_3^{\text{Lüders}}$ could be identified with the relevant temporal Tsirelson bound. However, as we will show, with a more general projective measurement scheme, violations of Eq. (1) for multilevel systems can exceed the qubit value.

Other than in an invasive scenario (where the algebraic maximum is trivially achieved, e.g., a classical device with memory or its quantum realization via positive-operator valued measures (POVMs) [8]), the only hint that a violation of Eq. (1) greater than $K_3^{\text{Lüders}}$ is possible has come in the recent work by Dakić *et al.* [20]. There, however, the excess violation was claimed to stem from correlations beyond quantum theory. In contrast, our excess violations are found within the standard framework of quantum theory and projective measurements. This we achieve by considering measurements on an N-level system that can project the state in one of M different subspaces, $2 \leq M \leq N$, with outcomes that are nevertheless associated with either $Q = +1$ or $Q = -1$. From a macroscopic-realist point of view, this leaves Eq. (1) unchanged. From a quantum perspective, however, the choice of M determines the state-update rule under projective measurement: For $M = 2$ the projection is onto one of two subspaces, corresponding to Lüders rule for dichotomic measurements [21], whereas $M = N$ is the case of a complete degeneracy-breaking measurement, as initially

proposed by von Neumann [22] (see also Ref. [23] for a discussion). These additional possibilities for state reduction are ultimately responsible for the increased violations.

In this Letter we use the example of a large spin precessing in a magnetic field to demonstrate that violations $K_3 > (3/2)$ are possible and that the algebraic bound $K_3 = 3$ can be reached. We then discuss the exact upper bounds for small $M \leq 5$, and how they may be obtained with few-dimensional systems with $N \leq 9$.

We discuss how a similar modification to the spatial Bell scenario does not lead to an increase in the Tsirelson bound for the corresponding Bell inequality [3]. Our results therefore reveal a stark contrast between spatial and temporal correlations. Furthermore, these results imply the utility of the LGIs with our extended measurement scheme as dimension witnesses [24], i.e., a certification of the minimum number of quantum levels an experimenter is able to manipulate, or in the discrimination of Lüders and von Neumann state-update rules [25].

Preliminary notions.—We consider measurements of a macroscopic property Q, which can take values ±1, on an N-level quantum system, with each level associated with a definite value of Q. From a macrorealist point of view, the fact that different levels are associated with the same value of Q is irrelevant: They may be considered as microscopically distinct states that have the same macroscopic property Q. Macrorealism and noninvasive measurability imply that at each instant of time, the system has a definite value of Q, which is independent of measurements previously performed on the system, and, therefore, that the bound for Eq. (1) in macrorealist theories remains the same.

From a quantum mechanical perspective, the fact that the system has more than two levels allows for many possible state-update rules. According to Lüders' rule [21], the state is updated as $\rho \mapsto \Pi_\pm \rho \Pi_\pm$, up to normalization, depending on the outcome of the measurement. On the opposite side, von Neumann's original proposal [22] is a state-update $\rho \mapsto \sum_k \Pi_\pm^{(k)} \rho \Pi_\pm^{(k)}$, where $\Pi_\pm^{(k)}$ are one-dimensional projectors. Both state-update rules are plausible, and the choice of the correct one depends on the particulars of the interaction between the system and the measurement apparatus (see Ref. [23] for a discussion).

More generally, we consider all possible intermediate cases, namely, state-update rules given by M different projectors, with $2 \leq M \leq N$, associated with either a $+1$ or -1 outcome. The correlation functions are therefore given by

$$C_{\beta\alpha} = \sum_{l,m} q_l q_m \text{Tr}\{\Pi_m U_{\beta\alpha} \Pi_l U_{\alpha 0} \rho_0 U_{\alpha 0}^\dagger \Pi_l U_{\beta\alpha}^\dagger\}, \quad (2)$$

where q_l represents the outcome ±1 associated with Π_l, ρ_0 is the initial state of the system, and $U_{\beta\alpha} = U(t_\beta - t_\alpha) = e^{-iH(t_\beta - t_\alpha)}$ is the unitary time-evolution operator for some Hamiltonian H.

A simple example.—Consider a quantum-mechanical spin of length j in a magnetic field oriented in the x direction. We write its Hamiltonian ($\hbar = 1$) as

$$H = \Omega J_x, \quad (3)$$

with Ω the level spacing and J_x the x component of the angular momentum operator. Let us choose to measure the spin in the z direction such that the measurement projectors are $\Pi_m^j = |m;j\rangle\langle m;j|$, with $|m;j\rangle$ eigenstates of the J_z operator. In this example, we only consider the von Neumann limit, $M = N = 2j + 1$, and choose the measurement values to be $q_m^j = 1 - 2\delta_{m,-j}$, such that the lowest energy state is associated with the value -1, and the rest with $+1$.

Calculating the correlation functions $C_{\beta\alpha}$ for this setup, several differences with the qubit case are immediately apparent. Most importantly, the correlation functions here depend on both times and not just their difference. As corollary, the correlation functions depend on the initial state. A further difference is that, for the projectively measured correlation functions discussed here, the order of the measurements $t_\beta > t_\alpha$ is important. This is not the case for $M = 2$, for which Fritz [8] has shown that, for arbitrary N, the projectively measured correlation functions are equal to the expectation value of the symmetrised product $\frac{1}{2}\{Q_j, Q_i\}$, where the operators Q have spectral decomposition $Q = \Pi_+ - \Pi_-$, with $\Pi_\pm$ the projectors associated with the eigenvalues ±1.

We initialize the system so that at time $t = 0$ it is in state $|\psi(t=0)\rangle = |-j;-j\rangle$ and set the measurement times as $\Omega t_1 = \pi$, $t_2 - t_1 = t_3 - t_2 = \tau$. For $N = 2$ we obtain the familiar qubit results [7]. For $N = 3$, the LGI parameter reads

$$K_3 = \frac{1}{16} + 2\cos(\Omega\tau) - \frac{5}{4}\cos(2\Omega\tau) + \frac{3}{16}\cos(4\Omega\tau), \quad (4)$$

which exhibits the key property in which we are interested —as we see in Fig. 1, this quantity shows a maximum of $K_3^{\max} = 1.7565$, clearly in excess of the Lüders bound.

Asymptotic limit.—Figure 1 further shows that the maximum value of K_3 for this model increases as a function of system size, N. In the limit $N \to \infty$, the maximum possible violation is $K_3^{\max} = 3$, as we now show. With measurement times $\Omega\tau = \frac{1}{2}\pi$, the correlation functions read (see the Supplemental Material [26])

$$C_{31} = -1; \qquad C_{21} = 1 - 2^{1-2j};$$
$$C_{32} = 1 - 2\frac{1}{2^{2j}} + 4\frac{1}{2^{4j}} - 2\frac{(4j)!}{4^{2j}[(2j)!]^2}. \quad (5)$$

The corresponding value of K_3 as a function of N is shown in Fig. 1. For finite N, this choice of measurement time does not give the maximum violation. However, this result
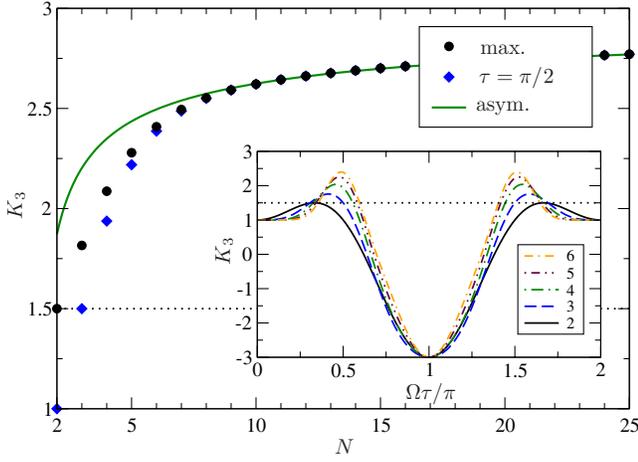
FIG. 1 (color online). The Leggett-Garg quantity K_3 for a spin of length $j = (N-1)/2$ precessing in a magnetic field with measurement times $\Omega t_1 = \pi$, $t_2 - t_1 = t_3 - t_2 = \tau$. The measurement is made with $M = N$ projectors (von Neumann scheme) in the z direction. Inset: K_3 as a function of measurement time τ for various values of N. For $N = 2$ the maximum is the familiar qubit or Lüders bound $K_3^{\max} = \frac{3}{2}$ (solid line). For $N = 3$, however, the maximum value is 1.7565, and this increases with increasing N. Main panel: The black circles show the maximum value $K_3^{\max}$ as a function of system size $N = 2j + 1$ for the spin precession model with measurement times as above. The blue diamonds show the value of K_3 with τ fixed $\Omega\tau = \pi/2$, and the solid line shows the asymptotic behavior $K_3^{\max} \sim 3 - \sqrt{2/\pi j}$. In the limit $N \to \infty$, $K_3^{\max}$ tends to the algebraic bound of 3.

serves to bound $K_3^{\max}$ and, for large j, the asymptotic behavior is

$$K_3 \to 3 - \sqrt{\frac{2}{\pi j}}. \qquad (6)$$

Thus, at least in the limit that the dimension of the system becomes infinite, the K_3 LGI can be violated by quantum mechanics all the way up to the algebraic bound.

Maximum violations.—While the precessing spin model reveals that violations greater than in the qubit case can occur, the violations for this system are *not* the maximum possible violations at a given N and M. Again, this is in contrast with the $M = 2$ case where the Rabi oscillation of the qubit provides the maximum violation.

To investigate the true maximum violations as a function of N and M, we combine two different methods. The maximum value for a given M can be obtained by means of the maximization method for temporal correlations based on semidefinite programming [9]. This method provides an upper bound valid for any N, which is attained for any $N \geq N_{\min}$. However, the exact value for $N_{\min}$ cannot be extracted from the solution, even though the method provides a state and a set of observables attaining the maximum quantum value (see the Supplemental Material [26]).

TABLE I. The maximum value of the LGI parameter K_3 as a function of system size N and number of projectors M. The leftmost results are from the semidefinite programming (SDP) approach, while the rest are from direct maximization with fixed N and M. Here the value assignments $q_m = 1 - 2\delta_{m,-j}$ were used. In general, the bound changes for different assignments, but except for the case $M = 6$, the above choice was found to give the maximum violation.

SDP		Maximization								
M	$K_3^{\max}$	M	N	$K_3^{\max}$	M	N	$K_3^{\max}$	M	N	$K_3^{\max}$
2	$\frac{3}{2}$	3	3	2.1547	4	4	2.3693	5	5	2.5166
3	2.211507	3	4	2.1736	4	5	2.3877	5	6	2.5312
4	2.454629	3	5	2.2115	4	6	2.4181	5	7	2.5459
5	2.579333	3	6	2.2115	4	7	2.4315	5	8	2.5506
6	2.656005	3	7	2.2115	4	8	2.4545	5	9	2.5545

We also pursue a complementary approach in which, for explicit values of N and M, we numerically maximize K_3 over time-evolution operators $U_{\beta\alpha}$ treated as general $N \times N$ unitary matrices. The results from these calculations are summarized in Table I and Fig. 2. We observe that the $M = 3$ and $M = 4$ bounds from semidefinite programming are saturated at relatively small system sizes, $N = 5$ and $N = 8$, respectively.

Temporal versus spatial correlations.—Leggett-Garg inequalities are often referred to as "Bell inequalities in time"; in addition, it is known that the Lüders bound for the n-term generalization, for even n, of the original Leggett-Garg inequality (1) coincides with the Tsirelson bound [9] for the corresponding Bell inequalities [27,28], and noncontextuality inequalities [29]. It is therefore a natural question whether the above general measurement scheme can provide excess quantum violation of Bell inequalities. The answer, however, is negative as can be easily deduced directly from the Tsirelson proof of the quantum bound [3]
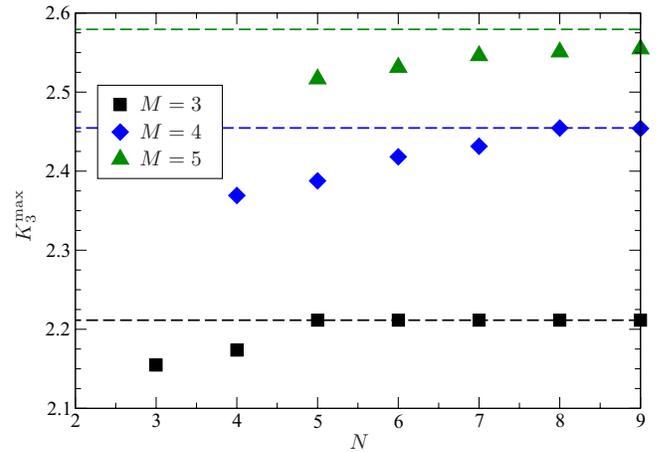

FIG. 2 (color online). A plot of the data in Table I. The maximum values for each M (from SDP) are shown as straight lines.

or by noticing that the commutativity of the measurements, even when performed sequentially as in contextuality tests, makes the postmeasurement state, and therefore which state-update rule is used, irrelevant.

Discussion.—We have shown that higher violations of the Leggett-Garg inequality are possible within the framework of standard quantum theory plus projective measurements. This is of fundamental importance since classical theories reproducing, or exceeding, the quantum correlations for temporal scenarios are conceivable and they do not violate any physical principle, as opposed to Bell scenarios where such classical theories involve faster-than-light communication between spacelike separated experiments. In fact, in a temporal scenario a classical device with memory, keeping track of the performed measurements and outcomes, can easily saturate the algebraic bound. However, such a device cannot be considered in Leggett-Garg tests since it contradicts the hypothesis of noninvasiveness of the measurement: The memory must be stored on a (possibly auxiliary) physical system. The same argument also applies to the quantum mechanical description of such a device, which is only possible with POVMs [8]. Such measurement schemes are, therefore, not meaningful in a Leggett-Garg test.

From an information-theoretic perspective, it is interesting to relate temporal correlations to the amount of information transmitted through sequential measurements [8]. While classical devices with memory, and their quantum counterparts based on POVMs, can easily saturate the algebraic bound $K_3 = 3$, the amount of information transmitted through sequential projective measurements, subjected to Lüders rule, has been proven to obey stricter bounds, independent of the system size [9]. Our analysis shows that degeneracy-breaking projective measurements, such as those in von Neumann's scheme, are able to transmit more information, which is encoded in the different evolution paths in the set of quantum states, and can give rise to perfect correlations (or anticorrelations) in the limit of an infinite number of projectors. This is in stark contrast with Bell inequalities, which do not show any higher violation when tested with more general types of quantum measurements and are typically saturated only in the framework of postquantum theories [6].

We stress that this analysis does not contradict the conclusions drawn in Ref. [9]; information-theoretic principles bounding the temporal correlations for projective measurements may still exist, but such principles must take into account the fact that the bound depends on the number of levels accessed via projective measurement.

An application of our results is that of a dimension witness [24]: An experimenter can certify that she is able to manipulate at least M levels of a quantum system, if she can violate the bound for $M - 1$. Obviously, the condition of projective measurement must also be verified. Notice that our dimension witnesses always involve the same

Leggett-Garg inequality and measurement scheme, in contrast to other proposals based on Bell [24] or non-contextuality [30] inequalities, and the prepare-and-measure scenario [31], where specific inequalities violated only by high-dimensional systems and involving more complex measurement schemes must be found.

A further interesting application is the discrimination between Lüders's and von Neumann's state-update rules [25], i.e., which one, if any, correctly represents the measurement scenario. A violation of the bound corresponding to $M = 2$ shows a contradiction with Lüders rule. Intermediate cases are possible and can also be investigated with our method.

Moreover, we hope that our results will be a catalyst for experimental investigation of higher-dimensional systems and the measurement of violations of the Leggett-Garg inequalities beyond those achievable either with a single qubit or, indeed, in a Bell scenario.

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