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Leggett–Garg-like Inequalities from a Correlation Matrix Construction

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Abstract: The Leggett–Garg Inequality (LGI) constrains, under certain fundamental assumptions, the correlations between measurements of a quantity Q at different times. Here, we analyze the LGI and propose similar but somewhat more elaborate inequalities, employing a technique that utilizes the mathematical properties of correlation matrices, which was recently proposed in the context of nonlocal correlations. We also find that this technique can be applied to inequalities that combine correlations between different times (as in LGI) and correlations between different locations (as in Bell inequalities). All the proposed bounds include additional correlations compared to the original ones and also lead to a particular form of complementarity. A possible experimental realization and some applications are briefly discussed.

Keywords: Leggett–Garg Inequality; Bell–Leggett–Garg Inequality; quantum correlations; quantum information; foundations of quantum mechanics

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1. Introduction

Leggett and Garg, in their seminal work [1], provided constraints on the correlations between measurements of a single quantity at different times. They showed that given the definition $C_{ij} \equiv \langle Q_i Q_j \rangle$ for the correlation between two measurements of a quantity Q at times t_i and t_j, the sum $|C_{12} + C_{23} + C_{34} - C_{14}|$ is bounded by 2 in any scenario that maintains "macrorealism" and "non-invasive measurability" [2]. Such a scenario represents the classical physics view of a macroscopic system, as a system that cannot be in two or more states at the same time and in which it is possible to measure the state with only an arbitrarily small perturbation of it. Determining whether the Leggett–Garg Inequality (LGI) holds for a given system assists in distinguishing between systems that obey this classical view and those that exhibit nonclassical behavior (in the particular sense linked to macrorealism). If a system violates the LGI, it necessarily exhibits nonclassical behavior. However, recent works have shown that the contrary is not always true, i.e., a system can satisfy the LGI but still violate macrorealism [3,4]. The initial motivation for the LGI was using this method to determine whether quantum coherence appears even in macroscopic systems. Later works focused on experimentally finding LGI violations in microscopic quantum systems using various measurement types such as ideal negative measurements [5]. A recent work by Shenoy et al. [6] presented the applicability of LGI in the area of quantum cryptography. They showed how the amount of the violation of the LGI indicated that a hacking attempt was made during the quantum key distribution protocol [7].

The LGI relates to the bounds on correlations of a single quantity measured typically on the same system at different times by the same party, in a manner that mathematically resembles the well-known Clauser–Horne–Shimony–Holt (CHSH) inequalities, providing bounds on the correlations between quantities measured typically on a bipartite system at two different locations by two different parties [8–10]. Similar to the "classical" LGI bound of 2, previous works have shown that under quantum assumptions, the same correlations are bounded by $2\sqrt{2}$ [11]. Here, we find more informative LGI bounds, tighter than $2\sqrt{2}$, by studying a more general definition for the correlations, which under certain conditions coincides with the common LGI correlations for quantum systems [12]. We apply a mathematical method that was recently proposed for finding richer bounds for the CHSH and other novel inequalities [13–16].

We show that maximal violations of the classical LGI bound in the newly found inequalities directly follow from the absence of correlations between an operator and itself at certain times. On the practical level, our results may allow one to better design quantum temporal correlations, but fundamentally, this highlights the necessity of certain noncommutativity between the measured operator and the Hamiltonian (see [17] for the broader consequences of noncommutativity and uncertainty).

In addition to their theoretical merits, we suggest that these tighter bounds may be beneficial for applied purposes as well, e.g., for devising quantum key distribution protocols (similar to [6]) or analyzing quantum metrological schemes (similar to [18]).

For completeness, we show in Appendix A that a different definition of the temporal correlation leads to other bounds.

2. Materials and Methods

We define the generalized correlation function $C(X,Y)$—for any two Hermitian operators X and Y—as

$$C(X,Y) = \frac{\frac{1}{2}\langle\{X,Y\}\rangle - \langle X\rangle\langle Y\rangle}{\Delta_X \Delta_Y}, \tag{1}$$

where $\{X,Y\}$ denotes the anticommutator, and $\Delta_X = \sqrt{\langle X^2\rangle - \langle X\rangle^2}$, $\Delta_Y = \sqrt{\langle Y^2\rangle - \langle Y\rangle^2}$ are the standard deviations. From the Schrödinger–Robertson uncertainty relation [19,20], it is easy to prove that this correlation is bounded between -1 and 1. If X and Y represent projective quantum measurements of values ± 1 with an expected value of 0, this correlation coincides with the symmetric correlation $\frac{1}{2}\langle\{X,Y\}\rangle$, which Fritz proposed as a quantum analog of the LGI correlation [12].

The motivation behind this generalized correlation definition is twofold: apart from the aforementioned fact that in the case of projective measurements it generalizes the standard symmetric correlation used for LGI, it is also widely used in quantum optics [21,22] and can be therefore readily generalized to the case of continuous variables.

After constructing the correlations matrix, we employ semi-positive definiteness conditions, similar to those in [13–16], to derive our Leggett–Garg-like inequalities.

3. Results

Here, we present four theorems and corresponding proofs entailing analytical bounds for the correlations between measurements of a quantum system at different times. Theorems 1–3 discuss elaborate Leggett–Greg-like inequalities describing constraints on generalized correlations of measurements at four consecutive measurement times. The measurement of a quantity Q at time t_i is described by the Hermitian operator Q_i. Theorem 1 is significant mainly because it provides a tighter bound than $2\sqrt{2}$, which is the known bound under typical quantum assumptions. Theorem 2 resembles the TLM inequality, which is a significant bound that was derived independently by Tsirelson, Landau, and Masanes [23–25]. The structure of the TLM inequality is characterized by the fact it that bounds products of correlations and not merely their sums as in other inequalities. Theorem 3 demonstrates a complementarity relation between all pairs of correlations of the four measurements.

Theorem 4 relates to a combination of the CHSH and LGI [26,27], where the constraints are on generalized correlations between quantities measured at two different times t_1 and t_2 by two parties, Alice and Bob, each in a different location. The two consecutive measurements of Alice (Bob) are represented by the Hermitian operators A_1 and A_2 (B_1 and B_2).

Theorem 1. *Elaborate Leggett–Garg-like inequality.*
Given four consecutive measurements, we define the generalized LGI parameter as

$$L = |C(Q_1, Q_2) + C(Q_2, Q_3) + C(Q_3, Q_4) - C(Q_1, Q_4)|. \tag{2}$$

The following holds

$$L \le 2\sqrt{1 + \sqrt{1 - \max\{C(Q_1, Q_3)^2, C(Q_2, Q_4)^2\}}}. \tag{3}$$

Proof of Theorem 1. Let C be the following correlation matrix

$$C = \begin{pmatrix} C(Q_{2i}, Q_{2i}) & C(Q_{2i}, Q_1) & C(Q_{2i}, Q_3) \\ C(Q_{2i}, Q_1) & C(Q_1, Q_1) & C(Q_1, Q_3) \\ C(Q_{2i}, Q_3) & C(Q_1, Q_3) & C(Q_3, Q_3) \end{pmatrix}, \tag{4}$$

where $i = 1, 2$. C is a positive semi-definite matrix, i.e., $C \succeq 0$ (see [14,15] for more details regarding the construction and properties of such matrices). Therefore, by the Schur complement condition for positive semi-definiteness,

$$\begin{pmatrix} 1 & C(Q_1, Q_3) \\ C(Q_1, Q_3) & 1 \end{pmatrix} \succeq \begin{pmatrix} C(Q_{2i}, Q_1) \\ C(Q_{2i}, Q_3) \end{pmatrix} \begin{pmatrix} C(Q_{2i}, Q_1) & C(Q_{2i}, Q_3) \end{pmatrix}. \tag{5}$$

Let $v_j^T = ((-1)^j, 1)$. Multiplying by v_j^T from the left and v_j from the right, the above inequality implies

$$2[1 + (-1)^j C(Q_1, Q_3)] \ge [C(Q_{2i}, Q_3) + (-1)^j C(Q_{2i}, Q_1)]^2. \tag{6}$$

For $j = i - 1$,

$$\begin{aligned} [C(Q_2, Q_1) + C(Q_2, Q_3)]^2 &\le 2[1 + C(Q_1, Q_3)] \\ [C(Q_4, Q_3) - C(Q_4, Q_1)]^2 &\le 2[1 - C(Q_1, Q_3)]. \end{aligned} \tag{7}$$

Since $C(Q_i, Q_j) = C(Q_j, Q_i)$ for any i and j, then

$$\begin{aligned} |C(Q_1, Q_2) + C(Q_2, Q_3)| &\le \sqrt{2[1 + C(Q_1, Q_3)]} \\ |C(Q_3, Q_4) - C(Q_1, Q_4)| &\le \sqrt{2[1 - C(Q_1, Q_3)]}. \end{aligned} \tag{8}$$

Using the triangle inequality on the two expressions in the left hand side of Equation (8), we derive the following

$$L \le 2\sqrt{1 + \sqrt{1 - C(Q_1, Q_3)^2}}. \tag{9}$$

By repeating the analytical derivation above for the following correlation matrix

$$\tilde{C} = \begin{pmatrix} C(Q_{2i-1}, Q_{2i-1}) & C(Q_{2i-1}, Q_4) & C(Q_{2i-1}, Q_2) \\ C(Q_{2i-1}, Q_4) & C(Q_4, Q_4) & C(Q_4, Q_2) \\ C(Q_{2i-1}, Q_2) & C(Q_4, Q_2) & C(Q_2, Q_2) \end{pmatrix}, \tag{10}$$

the multiplications by v_j^T and v_j give rise to:

$$2[1 + (-1)^j C(Q_4, Q_2)] \ge [C(Q_{2i-1}, Q_2) + (-1)^j C(Q_{2i-1}, Q_4)]^2. \tag{11}$$

From Equation (11), for the cases $i = j = 1$ and $i = j = 2$, the following inequality is derived using the triangle inequality

$$L \le 2\sqrt{1 + \sqrt{1 - C(Q_2, Q_4)^2}}. \tag{12}$$

Finally, Theorem 1 follows from Equations (9) and (12). Thus, we prove that given our assumptions, the generalized LGI parameter has a bound, which is tighter than $2\sqrt{2}$, and $2\sqrt{2}$ can be reached only if the correlations $C(Q_1, Q_3)$ and $C(Q_2, Q_4)$ are equal to 0. This result generalizes the known bound of $2\sqrt{2}$ for the LGI with projective measurements of values ± 1 [11]. □

Theorem 2. *Leggett–Garg-like inequality in the TLM form.*
Given four consecutive measurements,

$$\begin{aligned} &|C(Q_2,Q_1)C(Q_2,Q_3) - C(Q_4,Q_1)C(Q_4,Q_3)| \leq \\ &\sqrt{(1 - C(Q_2,Q_1)^2)(1 - C(Q_2,Q_3)^2)} + \sqrt{(1 - C(Q_4,Q_1)^2)(1 - C(Q_4,Q_3)^2)}. \end{aligned} \tag{13}$$

Proof of Theorem 2. Equation (5) implies

$$\begin{pmatrix} 1 - C(Q_{2i},Q_1)^2 & C(Q_1,Q_3) - C(Q_{2i},Q_1)C(Q_{2i},Q_3) \\ C(Q_1,Q_3) - C(Q_{2i},Q_3)C(Q_{2i},Q_1) & 1 - C(Q_{2i},Q_3)^2 \end{pmatrix} \succeq 0. \tag{14}$$

The determinant of the above matrix is nonnegative, and thus,

$$|C(Q_1,Q_3) - C(Q_{2i},Q_1)C(Q_{2i},Q_3)| \leq \sqrt{(1 - C(Q_{2i},Q_1)^2)(1 - C(Q_{2i},Q_3)^2)}. \tag{15}$$

For the cases $i = 1$ and $i = 2$, we obtain the following inequalities, respectively,

$$\begin{aligned} |C(Q_1,Q_3) - C(Q_2,Q_1)C(Q_2,Q_3)| &\leq \sqrt{(1 - C(Q_2,Q_1)^2)(1 - C(Q_2,Q_3)^2)} \\ |C(Q_1,Q_3) - C(Q_4,Q_1)C(Q_4,Q_3)| &\leq \sqrt{(1 - C(Q_4,Q_1)^2)(1 - C(Q_4,Q_3)^2)}. \end{aligned} \tag{16}$$

Finally, Theorem 2 is derived from the triangle inequality and Equation (16). The resulting inequality presents the TLM criterion for correlations between measurements at different times. □

Theorem 3. *Leggett–Garg-like inequality in the form of a complementarity relation.*
Given four consecutive measurements,

$$\left(\frac{L}{2\sqrt{2}}\right)^2 + \left(\frac{C(Q_1,Q_3)}{2\sqrt{2}}\right)^2 + \left(\frac{C(Q_2,Q_4)}{2\sqrt{2}}\right)^2 \leq 1. \tag{17}$$

Proof of Theorem 3. From Equation (9),

$$L^2 \leq 4\left(1 + \sqrt{1 - C(Q_1,Q_3)^2}\right). \tag{18}$$

Since $\sqrt{1-a} \leq 1 - a/2$ for $a \in [0,1]$, then

$$L^2 + 2C(Q_1,Q_3)^2 \leq 8, \tag{19}$$

and similarly we can derive from Equation (12),

$$L^2 + 2C(Q_2,Q_4)^2 \leq 8. \tag{20}$$

Theorem 3 is derived after summing Equations (19) and (20). This inequality demonstrates a complementarity relation between all six correlations of pairs from the four measurements. □

Theorem 4. *Elaborate Bell–Leggett–Garg-like inequality.*

For two consecutive measurements A_1 and A_2 of Alice and two consecutive measurements B_1 and B_2 of Bob, we define the generalized Bell–Leggett–Garg inequality parameter as

$$BLG = |C(A_1, A_2) + C(A_1, B_2) + C(B_1, B_2) - C(B_1, A_2)|. \tag{21}$$

The following holds

$$BLG \leq 2\sqrt{1 + \sqrt{1 - \max\{C(A_1, B_1)^2, C(A_2, B_2)^2\}}}. \tag{22}$$

Proof of Theorem 4. Let C_X be the following correlation matrix

$$C_X = \begin{pmatrix} C(X, X) & C(X, A_2) & C(X, B_2) \\ C(X, A_2) & C(A_2, A_2) & C(A_2, B_2) \\ C(X, B_2) & C(A_2, B_2) & C(B_2, B_2) \end{pmatrix}, \tag{23}$$

for $X \in \{A_1, B_1\}$. Following the analysis in the proof of Theorem 1, i.e., using the Schur complement condition for positive semi-definiteness and after multiplying by $v_j^T = ((-1)^j, 1)$ and v_j, we obtain

$$|C(X, B_2) + (-1)^j C(X, A_2)| \leq \sqrt{2[1 + (-1)^j C(A_2, B_2)]}. \tag{24}$$

For the two cases, ($X = A_1$ & $j = 0$) and ($X = B_1$ & $j = 1$), we obtain the following inequalities, respectively,

$$\begin{aligned} |C(A_1, B_2) + C(A_1, A_2)| &\leq \sqrt{2[1 + C(A_2, B_2)]} \\ |C(B_1, B_2) - C(B_1, A_2)| &\leq \sqrt{2[1 - C(A_2, B_2)]}. \end{aligned} \tag{25}$$

From the triangle inequality,

$$BLG \leq 2\sqrt{1 + \sqrt{1 - C(A_2, B_2)^2}}. \tag{26}$$

Similarly, by replacing the variables A_2 and B_2 by A_1 and B_1, respectively,

$$BLG \leq 2\sqrt{1 + \sqrt{1 - C(A_1, B_1)^2}}. \tag{27}$$

Finally, Theorem 4 is derived from Equations (26) and (27). □

An Example of a System That Upholds Our New Bounds

Here, we demonstrate Theorems 1–3 for a specific spin model [2,28], which is defined by the following Hamiltonian and observable

$$\begin{aligned} H &= \frac{\hbar\omega}{2}\sigma_x = \frac{\hbar\omega}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ Q &= \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \tag{28}$$

The time evolution of Q is

$$Q_t = \begin{pmatrix} \cos(\omega t) & -i\sin(\omega t) \\ i\sin(\omega t) & -\cos(\omega t) \end{pmatrix}; \tag{29}$$

therefore, according to Equation (1), the generalized correlation between two measurements of Q at times t and s is

$$C(Q_t, Q_s) = \cos\left(\omega(t - s)\right). \tag{30}$$

To demonstrate Theorem 1, for any four consecutive measurement times, we define $D1$ as the difference between our bound (the right hand side of Equation (3)) and the LGI parameter (Equation (2)). Thus, in our system,

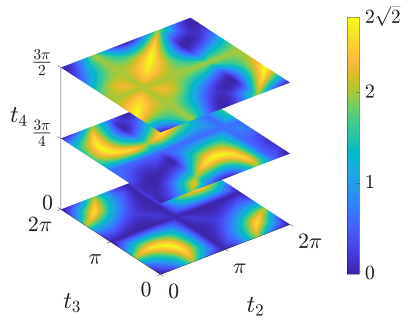
$$\begin{aligned} D1 = {} & 2\sqrt{1 + \sqrt{1 - \max\left\{\cos^2\left(\omega(t_1 - t_3)\right), \cos^2\left(\omega(t_4 - t_2)\right)\right\}}} \\ & - \left|\cos\left(\omega(t_1 - t_2)\right) + \cos\left(\omega(t_2 - t_3)\right) + \cos\left(\omega(t_3 - t_4)\right) - \cos\left(\omega(t_1 - t_4)\right)\right|. \end{aligned} \tag{31}$$

Similarly, to demonstrate Theorem 2, we define $D2$ as the difference between the right hand side and the left hand side of Equation (13); thus,

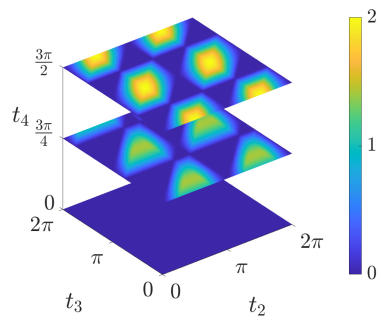
$$\begin{aligned} D2 = {} & \left|\sin(\omega(t_2 - t_1))\sin(\omega(t_2 - t_3))\right| + \left|\sin(\omega(t_4 - t_1))\sin(\omega(t_4 - t_3))\right| \\ & - \left|\cos(\omega(t_2 - t_1))\cos(\omega(t_2 - t_3)) - \cos(\omega(t_4 - t_1))\cos(\omega(t_4 - t_3))\right|. \end{aligned} \tag{32}$$

It can be shown numerically that $D1, D2 \geq 0$ for any t_1, t_2, t_3, and t_4 (see Figure 1a,b for a certain range of parameters). An example of a measurement time series in which the bound in Theorem 1 and the LGI parameter are both equal to $2\sqrt{2}$ is $t_1 = 0, t_2 = \pi/4, t_3 = \pi/2$, and $t_4 = 3\pi/4$.

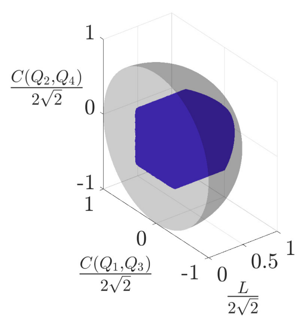
In Figure 1c, we demonstrate Theorem 3 by showing that the left hand side of Equation (17) is indeed smaller or equal to 1. To do so, we display all possible data points using the axes $L/2\sqrt{2}$, $C(Q_1, Q_3)/2\sqrt{2}$, and $C(Q_2, Q_4)/2\sqrt{2}$, and we note that they all reside within the unit sphere.



(**a**) Theorem 1 for our example.



(**b**) Theorem 2 for our example.



(**c**) Theorem 3 for our example.

Figure 1. Demonstration of Theorems 1–3 for our spin model. (**a**,**b**), the values of $D1$ and $D2$, respectively, both of which have a minimal value of 0, indicating Equations (3) and (13) are upheld. (**c**) The indigo area represents all data points, while the grey area represents the bounds of half of the unit sphere. All indigo points are within the gray area, indicating Equation (17) is upheld.

4. Discussion

In this manuscript, we studied generalizations of the LGI. We utilized a framework based on the quantum correlation matrix [13–15], which yielded a more detailed version of the LGI by incorporating additional correlations compared to the standard case. The results emphasize the major role of the positive-semidefinite correlation matrix in quantum mechanics not only in "spatial" scenarios but also in "temporal" ones. They also demonstrate a type of complementarity—in order for certain correlations to achieve their maximal values (left hand side of Equation (3)) others must vanish (those at the right hand side of Equation (3)).

We suggest that apart from its foundational and theoretical merits, the proposed bound may help in designing temporal correlations as well as the dynamics giving rise to them. They may also have practical implications in the area of quantum cryptography, as a possible generalization to existing encryption protocols that are based on LGI [6] or in the field of quantum metrology, possibly assisting approaches such as [18] or in LGI-based quantum computation assessment [29,30]. In addition, since there are known connections between correlation matrices and both classical [31] and quantum [32] Fisher information, the bounds derived in this manuscript can provide analogous bounds on elements of the Fisher information matrix.

Finally, the work presented in this manuscript provides concrete and measurable predictions; therefore, it can be verified in direct experiments. The system we provide as an example in the Section 3 is equivalent to the system, which was experimentally measured in [33], and the experimental results there are consistent with our bounds. In Appendix A, we propose an additional definition for the correlations and derive appropriate LGI-like bounds, which were not directly measured in previous experiments but can be either calculated or measured, e.g., via weak measurements [34].

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Appendix A

In this section, we discuss two subjects—another correlation definition and the significance of the underlying assumptions.

In principle, one can generalize the above results to the case of non-Hermitian quantum mechanics [35]. By defining the correlation $C(Q_i, Q_j)$ as the following complex correlation coefficient [14,15],

$$C(Q_i, Q_j) = \frac{\langle Q_i Q_j^\dagger \rangle - \langle Q_i \rangle \langle Q_j \rangle^\dagger}{\Delta_{Q_i} \Delta_{Q_j}}, \tag{A1}$$

and the complex-valued LGI parameter as

$$L = |C(Q_1, Q_2) + C(Q_2, Q_3) + C(Q_3, Q_4) - C(Q_1, Q_4)|, \tag{A2}$$

we obtain

$$
\begin{aligned}
&L \leq 2\sqrt{1+\sqrt{1-\max\left\{\Re^2[C(Q_1,Q_3)],\Re^2[C(Q_4,Q_2)]\right\}}} \\
&\left(\frac{L}{2\sqrt{2}}\right)^2+\left(\frac{\Re[C(Q_1,Q_3)]}{2\sqrt{2}}\right)^2+\left(\frac{\Re[C(Q_4,Q_2)]}{2\sqrt{2}}\right)^2 \leq 1,
\end{aligned}
\tag{A3}
$$

if $C(Q_2,Q_3) = C(Q_3,Q_2)$ or $[C(Q_1,Q_2) = C(Q_2,Q_1)$ & $C(Q_3,Q_4) = C(Q_4,Q_3)]$. The proofs of these bounds are similar to the proofs of Theorems 1 and 3.

As mentioned in the Section 3, the analysis of this manuscript yields a tighter LGI bound under the assumption of projective measurements with values ±1. We note that under different assumptions, the LGI parameter can reach the algebraic bound of 4 [36].

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