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Leggett-Garg inequalities and the geometry of the cut polytope

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The Bell and Leggett-Garg tests offer operational ways to demonstrate that non-classical behavior manifests itself in quantum systems, and experimentalists have implemented these protocols to show that classical worldviews such as local realism and macrorealism are false, respectively. Previous theoretical research has exposed important connections between more general Bell inequalities and polyhedral combinatorics. We show here that general Leggett-Garg inequalities are closely related to the cut polytope of the complete graph, a geometric object well-studied in combinatorics. Building on that connection, we offer a family of Leggett-Garg inequalities that are not trivial combinations of the most basic Leggett-Garg inequalities. We then show that violations of macrorealism can occur in surprising ways, by giving an example of a quantum system that violates the new “pentagon” Leggett-Garg inequality but does not violate any of the basic “triangle” Leggett-Garg inequalities.

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Keywords: Leggett-Garg inequality, cut polytope, macrorealism

Quantum theory offers a radical departure from the classical world, and this departure manifests itself operationally in the form of Bell [1] and Leggett-Garg inequalities (LGIs) [2]. A Bell inequality bounds the spatial correlations in any classical theory where observables have definite values and spacelike separated objects do not influence one another (*local realism* [3]). An LGI bounds the temporal correlations in any classical theory in which observables have definite values and measurement does not disturb the state (*macrorealism*). Since these theoretical insights, experimentalists have observed violations of local realism [4] and macrorealism [5] with quantum optical experiments. Recent theoretical evidence even suggests that measurement outcomes on biomolecules could violate an LGI [6].

The conventional setting for a Bell inequality involves two spacelike separated parties, say Alice and Bob, each of whom possess a quantum system A and B , respectively. Alice measures one of two dichotomic (± 1 -valued) observables A_1 or A_2 at her end, and Bob measures one of two dichotomic observables B_1 or B_2 at his end. The Clauser-Horne-Shimony-Holt (CHSH) Bell inequality [7] bounds the following sum of two-point correlation functions in any local realistic theory:

$$\langle A_1 B_1 \rangle + \langle A_1 B_2 \rangle + \langle A_2 B_1 \rangle - \langle A_2 B_2 \rangle \leq 2.$$

A bipartite quantum system in an entangled state can violate the above inequality, demonstrating that the local realistic picture of the universe is false.

Bell inequalities beyond the above conventional two-party, two-observable setting admit a rich mathematical structure. Peres showed that they correspond to the facets of a convex polytope, which he called the Bell polytope [8]. It is an example of a correlation polytope, which have been much studied, see for example Ref. [9] and the encyclopedic Ref. [10]. Avis *et al.* described a relationship between the Bell polytope and a projection of the cut

polytope [11, 12], a polytope which is isomorphic to the correlation polytope, and studied in depth in Ref. [10]. They were then able to offer 44,368,793 inequivalent tight Bell inequalities other than those of the CHSH form for the bipartite setting where each party measures ten dichotomic observables [11].

The conventional setting for an LGI involves a single party, say Quinn, who possesses a single quantum system. Quinn measures three dichotomic observables Q_1 , Q_2 , and Q_3 as his system evolves in time [18]. The LGI bounds a sum of two-time correlation functions in any macrorealistic theory:

$$\langle Q_1 Q_2 \rangle + \langle Q_2 Q_3 \rangle + \langle Q_1 Q_3 \rangle + 1 \geq 0. \quad (1)$$

Quinn can obtain the correlators $\langle Q_1 Q_2 \rangle$, $\langle Q_2 Q_3 \rangle$, and $\langle Q_1 Q_3 \rangle$ with many repetitions of one experiment where he measures all three observables, or he can obtain them with many repetitions of three different experiments where each experiment measures only the observables in a single correlator $\langle Q_i Q_j \rangle$. Note, for example, that if the system behaves according to the postulates of macrorealism, it should not matter in which way he obtains the correlators or even if he measures Q_2 while obtaining the correlator $\langle Q_1 Q_3 \rangle$. Any quantum system evolving according to a non-trivial, time-independent Hamiltonian leads to a violation of the above LGI [13].

The aim of the present paper is to go beyond the above conventional setting for a Leggett-Garg experiment and begin exploring the rich mathematical structure of LGIs with multiple measurements of dichotomic observables. The inequality in (1) is the simplest LGI, and it is a “triangle” LGI in the sense that it involves three observables and all three correlations between them. (This nomenclature will become more clear later when we explore richer LGIs.) Two works have already considered multiple measurements in LGIs [14, 15], but the first work [14] did not actually generate any “new” LGIs in the sense that

one can derive all inequalities found there by combining triangle LGIs. The aim of the second work [15] was to introduce extra measurements in order to address the “clumsiness loophole” in a Leggett-Garg experiment so it did not yield any new inequalities either. We also mention that another work considered the generalization of LGIs to higher-dimensional systems [16], but here we are only concerned with qubit observables.

In this Letter, we show that strong LGIs are equivalent to facet inequalities for the cut polytope of combinatorics [10]. This connection allows us to identify new classes of LGIs that are not merely combinations of triangle LGIs. The first interesting LGI that is not a trivial combination of triangle LGIs is a “pentagon” LGI involving the ten different pairwise correlations between five observables Q_1, \dots, Q_5 . We obtain other non-trivial inequalities for a higher number of observables by exploiting known results on the facets of the cut polytope. We also propose an experimental setup including five observables that violates the pentagon LGI, but in which the pairwise correlations of any three observables do not violate a triangle LGI. For this example, it is clear that the standard triangle Leggett-Garg test does not detect the presence of non-classicality, but a pentagon Leggett-Garg test does indeed detect non-classicality in the form of a violation.

We structure this work as follows. We first develop the connection between the LGIs and the cut polytope by reviewing some basic notions from polyhedral combinatorics. We then discuss our proposed experimental setup that violates the pentagon LGI but does not violate any triangle LGI.

LGIs and the cut polytope—A macrorealistic worldview implies that the set of joint probabilities accessible in any Leggett-Garg experiment involving n observables Q_1, \dots, Q_n is a convex polytope. An LGI corresponds to a valid inequality for this polytope, namely one that is satisfied by all vectors in the polytope. The strongest such inequalities are facets of the polytope and separate macrorealistic from non-macrorealistic behavior. Facets are those valid inequalities that cannot be obtained from a positive linear combination of other valid inequalities. They are the strongest inequalities in the following sense. A vector violating a (properly normalized) valid inequality that is not a facet will always provide a stronger violation of one of the (properly normalized) facets of which the valid inequality is a positive combination, hence our interest in finding new facets. We explain below that the Leggett-Garg polytope for n observables corresponds exactly to the cut polytope for a complete graph with n nodes.

We begin with some definitions from polyhedral combinatorics [10]. Suppose we have an integer $n \geq 2$ and a sequence (b_1, b_2, \dots, b_n) of integers. Let $b = \sum_{i=1}^n b_i$, $k = \sum_{i=1}^n |b_i|$ and note that b and k have the same parity. We can define a k -gonal inequality over real variables

x_{ij} , $1 \leq i < j \leq n$ using these integers:

$$\sum_{1 \leq i < j \leq n} b_i b_j x_{ij} \leq \left\lfloor \frac{b^2}{4} \right\rfloor. \quad (2)$$

Some special classes of the above inequality are of particular interest for us here. When b is even and some subset of the b_i sum to exactly $b/2$, the corresponding inequality is said to be of *negative type*. When b is odd and some subset of the b_i sum to exactly $\lfloor b/2 \rfloor$, the corresponding inequality is called *hypermetric*. Deza proved that each $2k$ -gonal inequality can be expressed as a positive combination of $(2k-1)$ -gonal inequalities (see, eg. [10]). So in this sense, there are no “new,” non-redundant inequalities for even values of b .

Now suppose $n = 3$. Then the hypermetric inequalities corresponding to the integer sequences $(1, 1, 1)$ and $(1, 1, -1)$ define, respectively, two types of triangle inequality:

$$x_{12} + x_{13} + x_{23} \leq 2, \quad (3)$$

$$x_{12} - x_{13} - x_{23} \leq 0. \quad (4)$$

The negative type inequality based on $(1, 1, 1)$ can easily be constructed by combining four of the first type of triangle inequality.

The set of all triangle inequalities defined on x_{ij} , $1 \leq i < j \leq n$ defines a full dimensional polytope, called the *semi-metric polytope*. The integer solutions to this set of inequalities are all 0/1-valued, and are called *cut vectors* because they are equivalent to the edge incidence vectors of cuts in the complete graph K_n [19]. The convex hull of the cut vectors is called the *cut polytope*. Hypermetric or negative type inequalities for which all $b_i = \pm 1$ are called *pure*. It is known that all pure hypermetric inequalities define facets of the cut polytope [10].

A vertex of the cut polytope represents the correlations between the values of n variables obtained in a single experiment, where each value is either 0 or 1. If there is a joint probability distribution over these n random variables and the experiment is repeated many times, then the average of the correlations obtained is a point in the convex hull of these vertices, i.e., a point in the cut polytope. Thus, the facets of the cut polytope collectively describe the correlations that are accessible in any macrorealistic theory. The triangle inequalities define all of the facets of the cut polytope for $n = 3$ and $n = 4$. The first new facet beyond the triangle inequalities is the pentagon inequality:

$$\sum_{1 \leq i < j \leq 5} x_{ij} \leq 6. \quad (5)$$

LGIs are typically expressed in terms of the expectations of ± 1 random variables, which we denote Q_1, Q_2, \dots, Q_n . The following relation allows us to convert the 0/1 values of the variables x_{ij} to the $+1/-1$

values for the two-time correlations $\langle Q_i Q_j \rangle$:

$$x_{ij} = \frac{1 - \langle Q_i Q_j \rangle}{2}. \quad (6)$$

We can then convert (2) to the following inequality:

$$\sum_{1 \leq i < j \leq n} b_i b_j \langle Q_i Q_j \rangle + \left[\frac{\sum_{i=1}^n b_i^2}{2} \right] \geq 0. \quad (7)$$

Because pure hypermetric inequalities give facets of the cut polytope, the inequality in (7) yields facets of the Leggett-Garg polytope when $b_i = \pm 1$. In this way, the triangle inequalities in (3) become the triangle LGIs [2]:

$$\langle Q_1 Q_2 \rangle + \langle Q_1 Q_3 \rangle + \langle Q_2 Q_3 \rangle + 1 \geq 0, \quad (8)$$

$$\langle Q_1 Q_2 \rangle - \langle Q_1 Q_3 \rangle - \langle Q_2 Q_3 \rangle + 1 \geq 0. \quad (9)$$

The second of the above inequalities is in fact the same as Bell's original inequality ([1], equation (15)). Since the cut polytope for $n = 4$ is completely defined by triangle inequalities, there are no new strong LGIs for correlations between 4 random variables. For $n = 5$ however, we obtain the pentagon LGI by rewriting (5) using (6):

$$\sum_{1 \leq i < j \leq 5} \langle Q_i Q_j \rangle + 2 \geq 0. \quad (10)$$

The inequalities (7), (8), (9) and (10), derived from hypermetric inequalities, define lower bounds on the two-time correlation functions in any macrorealistic theory.

Pentagon violation with no triangle violation—We provide a straightforward experimental setup that violates the pentagon LGI in (10), but does not violate any of the triangle LGIs. We assume that the system is noiseless and has vanishing Hamiltonian so that the dynamics are trivial. We choose as observables:

$$Q_1 \equiv \sigma_z, \quad Q_2 \equiv \sigma_\theta, \quad Q_3 \equiv \sigma_z, \quad Q_4 \equiv \sigma_\theta, \quad Q_5 \equiv \sigma_z,$$

where $\sigma_\theta \equiv \cos(\theta) \sigma_z + \sin(\theta) \sigma_x$ and σ_z and σ_x are Pauli operators. The inequality in (10) features ten two-time correlation functions. As stated before, Quinn can calculate these correlation functions in one experiment or he can calculate them with ten different experiments—the way in which he collects the correlation data should not matter according to the macrorealistic worldview. Also, assuming macrorealism, Quinn can choose to measure or not measure any of the observables Q_1, \dots, Q_5 while calculating the correlator $\langle Q_i Q_j \rangle$ because any of these measurements should not affect the state or its subsequent dynamics according to the macrorealistic worldview. So, for example, in the calculation of $\langle Q_1 Q_5 \rangle$, Quinn could measure Q_2 and this measurement should not affect the two-time correlation $\langle Q_1 Q_5 \rangle$ assuming macrorealism.

Figure 1 displays the ten two-time correlation experiments that together give a violation of the pentagon

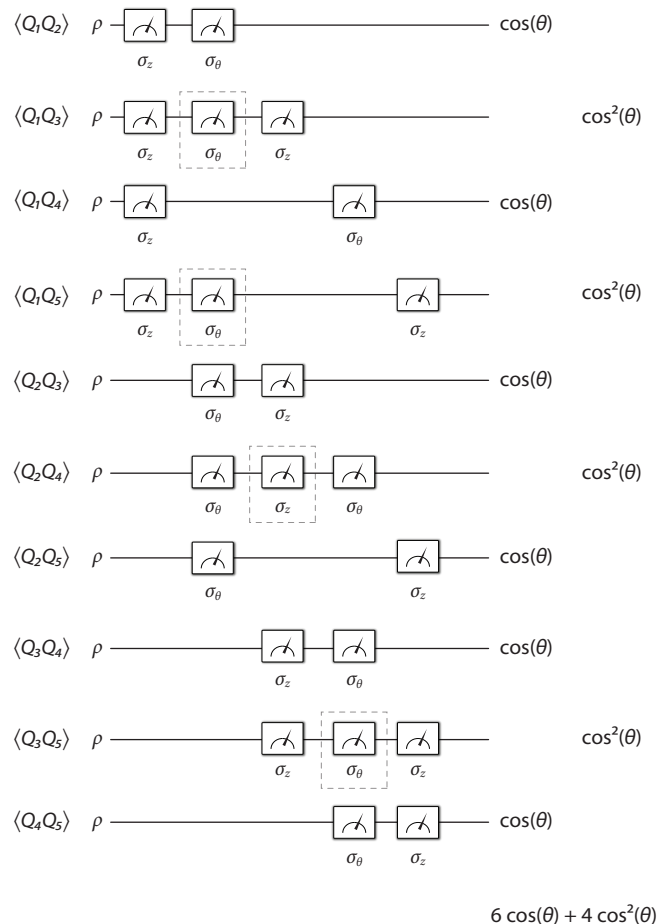


FIG. 1: The above figure displays the ten experiments that lead to a violation of the pentagon LGI. Additionally, any three experiments involving three distinct observables do not lead to a violation of the triangle LGI. We depict each two-time correlation function $\langle Q_i Q_j \rangle$ to the left of the corresponding experiment and display the value of each $\langle Q_i Q_j \rangle$ to the right of each experiment as a function of the angle θ . Boxed measurements indicate that the experimentalist Quinn performs the measurement but that its measurement results do not participate in the calculation of the corresponding two-time correlation function.

LGI. Additionally, any three of these experiments involving three distinct observables do not violate the triangle LGI. Below we prove that these statements hold. We first calculate several relevant quantities. We define the superoperator $\bar{\Delta}$ as a σ_z basis dephasing of a qubit with density operator ρ : $\bar{\Delta}(\rho) \equiv \frac{1}{2}(\rho + \sigma_z \rho \sigma_z)$, and $\bar{\Delta}_\theta$ as a σ_θ basis dephasing: $\bar{\Delta}_\theta(\rho) \equiv \frac{1}{2}(\rho + \sigma_\theta \rho \sigma_\theta)$. The following relation is useful: $\bar{\Delta}(\sigma_\theta) = \cos(\theta) \sigma_z$, and a similar relation holds by exploiting it: $\bar{\Delta}_\theta(\sigma_z) = \sigma_\theta \cos(\theta)$. If our input state is the maximally mixed state, then one can check that any two-time correlation function takes

the following form:

$$\langle Q_i Q_j \rangle = \frac{1}{2} \text{Tr} \{ Q_j \mathcal{N}(Q_i) \},$$

where \mathcal{N} is the map that represents the dynamics between measurement of Q_i and Q_j . Thus, if there is no measurement between measurement of Q_i and Q_j , then the two-time correlation function is

$$\langle Q_i Q_j \rangle = \frac{1}{2} \text{Tr} \{ Q_j Q_i \}.$$

If there is a measurement of σ_θ between the measurement of Q_i and Q_j , then

$$\langle Q_i Q_j \rangle = \frac{1}{2} \text{Tr} \{ Q_j \bar{\Delta}_\theta(Q_i) \}.$$

Using these ideas and the experiments in Figure 1, we calculate the following two-time correlation functions:

$$\begin{aligned} \langle Q_1 Q_2 \rangle &= \langle Q_1 Q_4 \rangle = \langle Q_2 Q_3 \rangle = \cos(\theta) \\ \langle Q_2 Q_5 \rangle &= \langle Q_3 Q_4 \rangle = \langle Q_4 Q_5 \rangle = \cos(\theta) \\ \langle Q_1 Q_3 \rangle &= \langle Q_1 Q_5 \rangle = \langle Q_2 Q_4 \rangle = \langle Q_3 Q_5 \rangle = \cos^2(\theta), \end{aligned}$$

Thus, for these experiments,

$$\sum_{1 \leq i < j \leq 5} \langle Q_i Q_j \rangle = 6 \cos(\theta) + 4 \cos^2(\theta).$$

Choosing θ so that $\cos(\theta) = -3/4$ leads to

$$\sum_{1 \leq i < j \leq 5} \langle Q_i Q_j \rangle = -9/4.$$

This is the smallest that the above ‘‘pentagon quantity’’ can be for any value of θ , and furthermore gives a violation of the pentagon LGI. One can also check that the two-time correlation functions in any three of these experiments involving three distinct observables never lead to a violation of the standard LGI because $2 \cos(\theta) + \cos^2(\theta) \geq -1$ for all θ .

Conclusion—The connection between LGIs and the cut polytope unveils a rich mathematical structure for Leggett-Garg tests with more than three observables. In particular, (2) combined with the mapping (6) gives families of new LGIs that are not trivial combinations of the original triangle LGIs. Our example in Figure 1 shows that it is possible to violate macrorealism in unexpected ways, e.g., by violating the pentagon LGI without violating any of the triangle LGIs. Future theoretical work could consider the effects of decoherence on these violations, similar to the study in Ref. [15]. One could also consider the maximal violations of LGIs possible in quantum mechanics. For Bell inequalities, the maximal violations are closely related to the ellipsope, a semidefinite relaxation of the cut polytope defined by the set of negative type inequalities [12]. In the case of LGIs, however,

an experimentalist is free to perform a measurement and ignore the outcomes: by exploiting the quantum Zeno effect [17] it then becomes possible in principle to avoid any meaningful constraint on the correlation functions. One could nonetheless restrict the experimentalist’s actions; perhaps the ellipsope arises from imposing some sensible restrictions.

Tobias Fritz recently informed us (private communication) that he had independently discovered the isomorphism between LGIs and the cut polytope. The authors gratefully acknowledge financial support from the Canada Research Chairs program, the Perimeter Institute, CIFAR, FQRNT’s INTRIQ, MITACS, NSERC, ONR grant N000140811249 and QuantumWorks. MMW was supported by an MDEIE (Québec) PSR-SIIRI international collaboration grant.

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- [18] Equivalently, Quinn could measure rotated observables if his system does not evolve in time.
- [19] The complete graph K_n is a graph with n vertices and $n(n-1)/2$ edges connecting all vertices to each other. A (edge) cut of K_n is defined by any subset S of its vertices, and consists of those edges joining a vertex of S to a vertex not in S . The edge incidence vector of a cut is a binary vector of size $n(n-1)/2$. A component of the vector is “zero” if an edge is not present in the cut, and it is “one” otherwise. There are 2^{n-1} such vectors.