Letter

Optimal and tight Bell inequalities for state-independent contextuality sets

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Two fundamental quantum resources, nonlocality and contextuality, can be connected through Bell inequalities that are violated by state-independent contextuality (SI-C) sets. These Bell inequalities allow for applications that require simultaneous nonlocality and contextuality. However, for existing Bell inequalities, the nonlocality produced by SI-C sets is very sensitive to noise. This precludes experimental implementation. Here we identify the Bell inequalities for which the nonlocality produced by SI-C sets is optimal, i.e., maximally robust to either noise or detection inefficiency, for the simplest SI-C [S. Yu and C. H. Oh, Phys. Rev. Lett. **108**, 030402 (2012)] and Kochen-Specker sets [A. Cabello *et al.*, Phys. Lett. A **212**, 183 (1996)] and show that, in both cases, nonlocality is sufficiently resistant for experiments. Our work enables experiments that combine nonlocality and contextuality and therefore paves the way for applications that take advantage of their synergy.

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Introduction. Bell nonlocality [1–3] and Kochen-Specker (KS) contextuality [4–6] are two fundamental quantum resources that are crucial for quantum information processing. Applications such as device-independent quantum key distribution [7–9] require nonlocality. On the other hand, certain schemes for universal quantum computation [10,11], quantum computation tasks with quantum advantage [12], and methods for benchmarking quantum computers [13,14] need contextuality. In addition, applications such as communication complexity [15,16], certification of quantum devices [17–19], and dimension witnessing [20,21] require either nonlocality or contextuality, depending on the task.

Here we address the problem of *combining* nonlocality and contextuality in the same experiment. This will allow us to tackle tasks that cannot be accomplished using either nonlocality or contextuality individually. To this end, we consider the scenario depicted in Fig. 1, involving three nodes (Alice, Bob, and Charlie). A source of entangled pairs of particles is placed between Alice and Bob, which they use to produce nonlocal correlations. Furthermore, we assume that the measurements that Bob performs are nondemolition projective (also known as ideal [22]) measurements and that Charlie performs additional measurements on Bob's particle [23–29] (see Fig. 1). We aim at producing contextuality between Bob and Charlie using the same state and measurements that Bob uses for producing nonlocality with Alice. We refer to this target as simultaneous nonlocality and contextuality (SNC).

The straightforward application of SNC is employing two protocols with quantum advantage in the same experiment. These could be, for example, nonlocality-based secret communication [7] and a contextuality-based communication complexity protocol with quantum advantage [16]. In addition, SNC is important by itself as there are applications that require both nonlocality and contextuality to achieve tasks that none of them can accomplish individually [28]. For example, combining nonlocality- and contextuality-based self-testing [17,18] might facilitate certification of quantum transformations produced by Bob's device [30]. Finally, a third motivation for SNC is investigating the connections between nonlocality and contextuality [31].

Simultaneous nonlocality and contextuality cannot be produced by simply combining the violation of the simplest Bell inequality, the Clauser-Horne-Shimony-Holt inequality [32], between Alice and Bob, and the violation of the simplest noncontextuality inequality, the Klyachko-Can-Binicioğlu-Shumovsky inequality [33], between Bob and Charlie. The reason is that, in this case, there is a fundamental trade-off between nonlocality and contextuality [24,25,29]. However, it has been recently shown [34] that SNC is possible if all parties choose their measurements from any state-independent contextuality (SI-C) set [35,36]. A SI-C set contains two-outcome observables represented by rank-one projectors and produces contextual correlations (i.e., violates a given noncontextuality inequality) no matter what the initial quantum state is. In particular, a SI-C set produces contextuality also when the initial state is mixed, as it is the case for the reduced state of Bob's particle before he performs his measurement (see Fig. 1). State-independent contextuality sets have been shown

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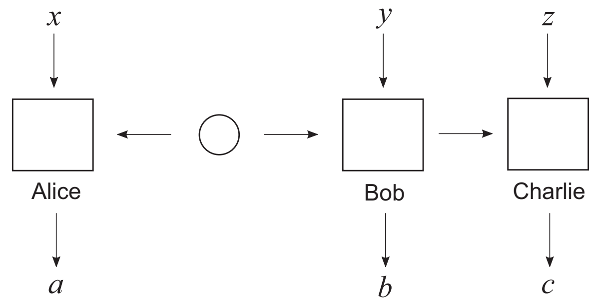
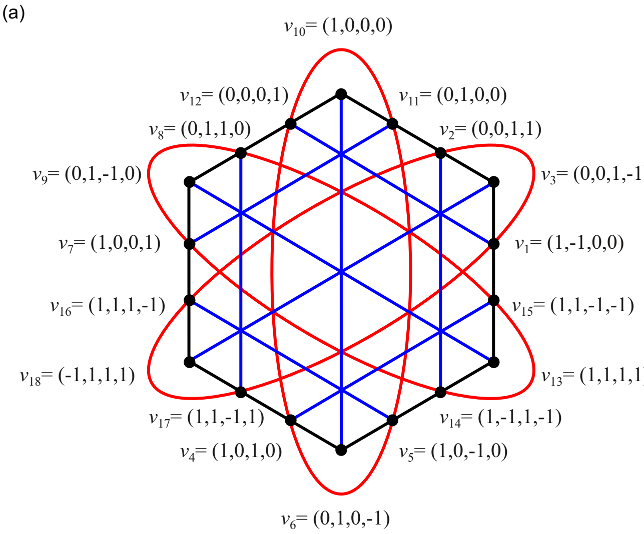


FIG. 1. Simultaneous nonlocality and contextuality. If Alice and Bob share a source of pairs of maximally entangled qudits, $x, y, z \in S$, and S is a SI-C set (and thus $a, b, c \in \{0, 1\}$), then the parties produce simultaneously Bell nonlocality between Alice and Bob and contextuality between Bob and Charlie.

(a)



(b)

	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	**0**	−2	−2	0	0	1	1	0	0	1	1	−2	−2	1	−2	−2	−2	1
0	−2	**0**	−2	1	0	0	0	0	1	−2	−2	1	1	−2	1	−2	−2	1
0	−2	−2	**0**	0	1	0	0	1	0	−2	−2	1	−2	1	−2	1	1	−2
0	0	1	0	**0**	−2	−2	0	0	1	1	−2	−2	1	1	−2	1	−2	−2
0	0	0	1	−2	**0**	−2	0	1	0	1	−2	−2	−2	−2	1	−2	1	1
0	1	0	0	−2	−2	**0**	1	0	0	−2	1	1	−2	−2	1	1	−2	−2
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0	0	1	0	1	0	0	−2	−2	**0**	−2	1	−2	−2	1	1	−2	1	−2
0	1	−2	−2	1	1	−2	1	−2	−2	**0**	−2	−2	0	0	1	1	0	0
0	1	−2	−2	−2	−2	1	−2	1	1	−2	**0**	−2	1	0	0	0	1	0
0	−2	1	1	−2	−2	1	1	−2	−2	−2	−2	**0**	0	1	0	0	0	1
0	−2	1	−2	1	−2	−2	1	1	−2	0	1	0	**0**	−2	−2	0	1	0
0	1	−2	1	1	−2	−2	−2	−2	1	0	0	1	−2	**0**	−2	0	0	1
0	−2	1	−2	−2	1	1	−2	−2	1	1	0	0	−2	−2	**0**	1	0	0
0	−2	−2	1	1	−2	1	−2	1	−2	1	0	0	0	0	1	**0**	−2	−2
0	−2	−2	1	−2	1	−2	1	−2	1	0	1	0	1	0	0	−2	**0**	−2
0	1	1	−2	−2	1	−2	−2	1	−2	0	0	1	0	1	0	−2	−2	**0**

FIG. 2. (a) KS18 and its graph of compatibility. Each vector v_i of KS18 is represented by a black node. Orthogonal vectors, which correspond to compatible observables, are represented by adjacent nodes. Nodes along the same straight line (or ellipse) represent mutually adjacent nodes. Same color nodes (edges) are structurally equivalent (see the Supplemental Material [22]). (b) Bell operator I^t_{KS18}. The Bell inequality $I^t_{\mathrm{KS18}} \leqslant 8$ is tight and is maximally violated by the KS18 correlations. The coefficients of I^t_{KS18} are presented using a matrix of the form (5). Color coding is used to emphasize that the coefficients in I^t_{KS18} share the same symmetries as the graph shown in (a). The entries with white background correspond to graph nodes and edges shown in (a). The coefficients of the entries with white background are also color coded. The coefficients associated with the corresponding edges have the same color as used in (a) (red, blue, and black). The coefficients associated with nonadjacent nodes [not shown in (a)] have entries with three different backgrounds (orange, violet, and cyan), one for each of the three orbits of nonadjacent nodes in (a) (see the Supplemental Material [22]).

experimentally [37–39] and can be considered fundamental quantum resources on their own.

The first SI-C set identified had 117 observables in dimension $d = 3$ and was used by Kochen and Specker to prove the KS theorem of impossibility of hidden variables [4]. State-independent contextuality sets that have the properties needed to prove the KS theorem are called KS sets (see the Supplemental Material [22]). Recently, it has been shown [40] that the simplest KS set has 18 observables in dimension $d = 4$ [41]. This set, here called KS18, is shown in Fig. 2(a). The optimal (i.e., maximally violated by KS18, for any state, including states with an arbitrary degree of noise) and tight noncontextuality inequalities (i.e., separating the set of noncontextual and contextual correlations) for KS18 are known [35,42,43].

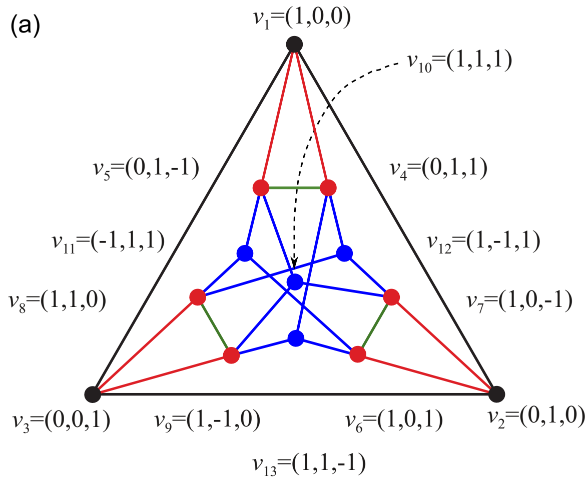
While any KS set is a SI-C set, not any SI-C set is a KS set (see the Supplemental Material [22]). The simplest [44,45] SI-C set is the one with 13 observables in dimension $d = 3$ found by Yu and Oh [46] and shown in Fig. 3(a). The Yu-Oh set is not a KS set [22]. The optimal and tight noncontextuality inequalities for the Yu-Oh set are also known [43].

The correlations produced by measuring any SI-C set in dimension d on a two-qudit maximally entangled state violate a Bell inequality constructed from the SI-C set [41]. However, such inequalities are neither optimal (in this case meaning maximally resistant to either noise or detection inefficiency [47]) nor tight Bell inequalities (i.e., separating the set of local and nonlocal correlations [48]). Moreover, these inequalities do not allow for experimental Bell tests because nonlocality with respect to them is very sensitive to noise, which prevents experimental implementations and in particular those with spacelike separation. On the other hand, tightness is important for both fundamental and practical reasons [49–53].

The fact that the optimal and tight Bell inequalities are not known for any SI-C set contrasts with the fact that, as it was pointed out before, the optimal and tight noncontextuality inequalities for KS18 and the Yu-Oh set were already identified. This means that, in the scenario shown in Fig. 1, the optimal witnesses for detecting contextuality between Bob and Charlie using the most fundamental SI-C sets are known, but the optimal witnesses for detecting nonlocality between Alice and Bob are still missing.

The aim of this work is to identify the optimal and tight Bell inequalities for the correlations produced by measuring KS18 and the Yu-Oh set on maximally entangled states. Hereafter, we will refer to these correlations as KS18 correlations and Yu-Oh correlations, respectively.

Our motivation roots, first, in having Bell inequalities that can be exploited and deployed in experiments requiring spacelike separation and that enable the development of SNC and its



(b)

	−1	−1	−1	−1	−1	−1	−1	−1	−1	3	3	3	3
−1	**0**	0	0	−1	−1	1	1	1	1	0	0	0	0
−1	0	**0**	0	1	1	−1	−1	1	1	0	0	0	0
−1	0	0	**0**	1	1	1	1	−1	−1	0	0	0	0
−1	−1	1	1	**0**	0	0	0	0	0	2	2	−2	−2
−1	−1	1	1	0	**0**	0	0	0	0	−2	−2	2	2
−1	1	−1	1	0	0	**0**	0	0	0	2	−2	2	−2
−1	1	−1	1	0	0	0	**0**	0	0	−2	2	−2	2
−1	1	1	−1	0	0	0	0	**0**	0	2	−2	−2	2
−1	1	1	−1	0	0	0	0	0	**0**	−2	2	2	−2
3	0	0	0	2	−2	2	−2	2	−2	**0**	−3	−3	−3
3	0	0	0	2	−2	−2	2	−2	2	−3	**0**	−3	−3
3	0	0	0	−2	2	2	−2	−2	2	−3	−3	**0**	−3
3	0	0	0	−2	2	−2	2	2	−2	−3	−3	−3	**0**

FIG. 3. (a) Yu-Oh set and its graph of compatibility. Each vector v_i of the Yu-Oh set is represented by a node. Orthogonal vectors, which correspond to compatible observables, are represented by adjacent nodes. Same color nodes (edges) are equivalent (see the Supplemental Material [22]). (b) Bell operator $I^t_{\text{Yu-Oh},V}$. The Bell inequality $I^t_{\text{Yu-Oh},V} \leqslant 12$ is tight and provides maximum resistance to noise for the Yu-Oh correlations. The coefficients of $I^t_{\text{Yu-Oh},V}$ are presented with the aid of a matrix of the form (5). Color coding is used to emphasize that the coefficients in $I^t_{\text{Yu-Oh},V}$ share the same symmetries as the graph shown in (a). The entries with white background correspond to graph nodes and edges. The coefficient associated with each of the nodes (edges) has the same color as used in (a) (red, blue, black, and green). The coefficients associated with nonadjacent nodes have entries with five different backgrounds (brown, violet, cyan, orange, and magenta), one for each of the five orbits of nonadjacent nodes [not shown in (a)] (see the Supplemental Material [22]).

applications. Second, we are motivated by the fact that optimal and tight Bell inequalities for SI-C sets are by themselves fundamental. On the one hand, they provide the optimal way of using a fundamental quantum resource (a SI-C set) for producing a fundamental quantum effect (nonlocality). On the other hand, they allow proving Bell's theorem [1] through the violation of Bell inequalities inspired by the KS theorem [4], thus connecting these two fundamental theorems.

Methods. The set of local correlations for the Bell scenario with two parties, m measurement settings, and two outcomes, called the $(2, m, 2)$ Bell scenario, is a polytope, called the local polytope, that has 2^{2m} vertices [48]. For the KS18 correlations, $m = 18$. For the Yu-Oh correlations, $m = 13$. This makes finding optimal and tight Bell inequalities difficult (see the Supplemental Material [22]).

To address this, we developed a three-step approach. In the first step, we identify Bell inequalities for which the nonlocality of the KS18 or Yu-Oh correlations has high resistance to noise or detection inefficiency. In the second step, we verify whether these inequalities are tight and if not we use them to construct tight inequalities. In the third step, we verify whether the resulting inequalities are maximally robust to either white noise or detection inefficiency, respectively.

In the first step, we implement a numerical technique based on Gilbert's algorithm for quadratic minimization [54]. This iterative algorithm minimizes the distance between a given matrix of correlations and the local polytope and yields a Bell inequality [55–57] (see the Supplemental Material [22] for details).

Depending on the type of robustness we want, we adopt a different approach. To obtain Bell inequalities with high resistance to white noise, we assume that the state shared by Alice and Bob is of the form

$$\rho = V|\psi\rangle\langle\psi| + (1-V)\frac{\mathbb{1}}{d^2}, \tag{1}$$

where $|\psi\rangle = \frac{1}{\sqrt{d}}\sum_{j=1}^{d}|jj\rangle$, $\mathbb{1}$ is the identity matrix, d is the dimension of the local subsystems ($d = 4$ and 3 for the KS18 and Yu-Oh correlations, respectively), and V is called the visibility. For any state of the form (1), the joint probability that Alice obtains outcome 1 for measurement Π_i (with possible outcomes 0 and 1) on her particle and Bob obtains the outcome 1 for measurement Π_j on his particle is

$$P_\rho(\Pi_i^A = \Pi_j^B = 1) = VP_{|\psi\rangle}(\Pi_i^A = \Pi_j^B = 1) + (1-V)\frac{1}{d^2}. \tag{2}$$

Similarly, the marginal probability that each of the parties obtains outcome 1 for measurement Π_i is

$$\begin{aligned} P_\rho(\Pi_i^A = 1) &= VP_{|\psi\rangle}(\Pi_i^A = 1) + (1-V)\frac{1}{d}, \\ P_\rho(\Pi_i^B = 1) &= VP_{|\psi\rangle}(\Pi_i^B = 1) + (1-V)\frac{1}{d}. \end{aligned} \tag{3}$$

For a given Bell inequality, we denote by V_{crit} the minimum value of V required to violate the inequality with the state (1).

To obtain Bell inequalities resistant to detection inefficiency, we assume that the source of pairs is heralded, the initial state is $|\psi\rangle$, and each of the parties assigns the outcome 0 when they fail to detect the particle [47]. Then

$$\begin{aligned} P^\eta(\Pi_i^A = \Pi_j^B = 1) &= \eta^2 P_{|\psi\rangle}(\Pi_i^A = \Pi_j^B = 1), \\ P^\eta(\Pi_i^A = 1) &= \eta P_{|\psi\rangle}(\Pi_i^A = 1), \\ P^\eta(\Pi_j^B = 1) &= \eta P_{|\psi\rangle}(\Pi_j^B = 1), \end{aligned} \tag{4}$$

where η is the detection efficiency; η it is assumed to be the same for all parties, measurements, and outcomes. For each correlation (i.e., state and measurements) violating a Bell inequality, there is a critical value of the detection efficiency η_{crit} above which local models cannot simulate the quantum correlations [47].

At the end of the first step, we have Bell inequalities with respect to which the KS18 or Yu-Oh correlations are robust to either noise or detection inefficiency. In the second step, we check whether these inequalities are tight. To this end, we collect all the vertices that saturate the local bound and form the largest set of affinely independent vectors. If the length of the affinely independent set is D, then they span a vectorial subspace of dimension $D-1$ (the polytope is in $\mathbb{R}^D$), hence a facet of the local polytope so the Bell inequality is tight [50,58].

However, in most cases the Bell inequalities obtained after the first step are not tight. Then we use them to obtain tight inequalities. For that, we exploit three facts. (i) When the inequalities obtained after the first step are written using the Collins-Gisin parametrization [59] (explained below), their coefficients display symmetries that allow us to reduce the number of independent coefficients. (ii) The vertices of the local polytope that saturate the local bound have an orthogonal subspace of dimension 1. Therefore, the linear combination of all these vertices must be a vector with at most one component equal to zero. Otherwise there would be at least two linearly independent vectors that are orthogonal to all the vertices, leading to an orthogonal subspace of at least dimension 2. (iii) A facet of a polytope in $\mathbb{R}^D$ must at least be saturated by D vertices. Otherwise, this facet could not contain D affinely independent vectors [60,61]. (See the Supplemental Material [22] for details.)

Finally, the third step of our method consists in proving that the inequalities obtained after the second step are optimal with respect to white noise or detection efficiency. In order to do so, we identify local models that, for the critical values of detection efficiency η_{crit} and visibility V_{crit}, reproduce the KS18 or Yu-Oh correlations. (See the Supplemental Material [22] for details.)

The Collins-Gisin parametrization follows from the fact that any Bell inequality with two-outcome measurements can be written as $I \leqslant \mathcal{L}$, with $I = \sum_{x,y} c(\Pi_x^A = \Pi_y^B = 1)P(\Pi_x^A = \Pi_y^B = 1) + \sum_x c(\Pi_x^A = 1)P(\Pi_x^A = 1) + \sum_y c(\Pi_y^B = 1)P(\Pi_y^B = 1)$, where the coefficients can be arranged in a matrix as

$$\left(\begin{array}{c|ccc} & c(\Pi_1^A = 1) & \cdots & c(\Pi_m^A = 1) \\ \hline c(\Pi_1^B = 1) & c(\Pi_1^A = \Pi_1^B = 1) & \cdots & c(\Pi_m^A = \Pi_1^B = 1) \\ \vdots & \vdots & \ddots & \vdots \\ c(\Pi_m^B = 1) & c(\Pi_1^A = \Pi_m^B = 1) & \cdots & c(\Pi_m^A = \Pi_m^B = 1) \end{array}\right) \tag{5}$$

and $\mathcal{L}$ is the upper bound of I for local models.

Results. Using the methods described before, we have obtained five Bell inequalities: two optimal and tight Bell inequalities for the Yu-Oh correlations and two optimal and one tight Bell inequalities for the KS18 correlations. The tight inequalities for the (2,13,2) Bell scenario are

$$I^t_{\text{Yu-Oh},V} \leqslant 12, \tag{6}$$

$$I^t_{\text{Yu-Oh},\eta} \leqslant 4, \tag{7}$$

where $I^t_{\text{Yu-Oh},V}$ is given in Fig. 3(b) and $I^t_{\text{Yu-Oh},\eta}$ in the Supplemental Material [22]. The subindex Yu-Oh indicates the correlations used to obtain the inequality. The subindex V or η indicates that the correlations are maximally resistant to either noise or detection inefficiency, respectively. The superindex t indicates that the inequality is tight. The Yu-Oh correlations yield

$$I^t_{\text{Yu-Oh},V} = \tfrac{46}{3} \approx 15.333, \tag{8}$$

$$I^t_{\text{Yu-Oh},\eta} = \tfrac{86}{9} \approx 9.555. \tag{9}$$

The critical visibility for $I^t_{\text{Yu-Oh},V}$ and the critical detection efficiency for $I^t_{\text{Yu-Oh},\eta}$ are

$$V_{\text{crit}} = 0.7917, \tag{10}$$

$$\eta_{\text{crit}} = 0.8441, \tag{11}$$

respectively, which, on the one hand, are a significant improvement compared to the values in [34], namely, $V_{\text{crit}} = 0.9578$ and $\eta_{\text{crit}} = 0.9710$, respectively (see the Supplemental Material [22] for details), and, on the other hand, are within the reach of currently attainable visibilities in experiments with high-dimensional systems [62–66] and current detection efficiencies for photons [67].

We have also obtained three Bell inequalities for the (2,18,2) Bell scenario,

$$I^t_{\text{KS18}} \leqslant 8, \tag{12}$$

$$I_{\text{KS18},V} \leqslant 12, \tag{13}$$

$$I_{\text{KS18},\eta} \leqslant 0, \tag{14}$$

where I^t_{KS18} is given in Fig. 2(b) and $I_{\text{KS18},V}$ and $I_{\text{KS18},\eta}$ are given in the Supplemental Material [22]. The KS18 correlations yield

$$I^t_{\text{KS18}} = \tfrac{45}{4} = 11.25, \tag{15}$$

$$I_{\text{KS18},V} = \tfrac{73}{4} = 18.25, \tag{16}$$

$$I_{\text{KS18},\eta} = \tfrac{27}{4} = 6.75. \tag{17}$$

The critical visibility for $I_{\text{KS18},V}$ and the critical detection efficiency for $I_{\text{KS18},\eta}$ are

$$V_{\text{crit}} = 0.8169, \tag{18}$$

$$\eta_{\text{crit}} = 0.8421, \tag{19}$$

respectively, which are a significant improvement over the values in [34], namely, $V_{\text{crit}} = 0.9317$ and $\eta_{\text{crit}} = 0.9428$, respectively (see the Supplemental Material [22] for details). Moreover, $I_{\text{KS18},\eta} \leqslant 0$ allows for loophole-free experiments with nonheralded sources [47].

Finding tight Bell inequalities for the KS18 correlations proved to be more challenging due to the complexity of the corresponding local polytope. However, we obtained one tight inequality $I^t_{\mathrm{KS18}} \leqslant 8$. This inequality displays an interesting feature: Its quantum bound (i.e., the highest possible value allowed by quantum mechanics) matches the value attained by the KS18 correlations. This is remarkable because it proves that the KS18 correlations are in the boundary of the set of quantum correlations, which means that they are not only nonlocal, but also extremal [30]. Extremality has been recognized as the key feature for nonlocal correlations to allow for device-independent quantum key distribution [2,68] and self-testing of quantum devices [19]. (See the Supplemental Material [22] for further details on device-independent applications of the KS18 and Yu-Oh correlations.)

Finally, as shown in Figs. 2 and 3, two of the tight Bell operators I^t_{KS18} and $I^t_{\mathrm{Yu\text{-}Oh},V}$, respectively, display the same (highly nontrivial) symmetries as the graph of compatibility of the corresponding set of local measurements (see the Supplemental Material [22]). This is surprising and requires further investigation, since, *a priori*, we do not expect any facet of the local polytope to be related to the graph of compatibility of a SI-C set.

Conclusion. Using a three-step method, we have obtained Bell inequalities that are optimal (maximally resistant to either noise or detection inefficiency) for correlations produced by maximally entangled states and KS18 (the simplest KS set in quantum mechanics) and the Yu-Oh set (the simplest SI-C set). They fundamentally connect the theorems of Bell, and Kochen and Specker, allow us to perform Bell tests with SI-C sets and spacelike separation and achieve simultaneous Bell nonlocality (with spacelike separation) and contextuality (with timelike separation). Therefore, they pave the way to tasks requiring both resources simultaneously and, more importantly, to tasks that cannot be accomplished with each of the resources individually. We have demonstrated that the KS18 correlations maximally violate the Bell inequality $I^t_{\mathrm{KS18}} \leqslant 8$ and can be used for device-independent quantum key distribution. Moreover, they allow for Bell self-testing while KS18 can also be used for certification with sequential measurements (Bob and Charlie in Fig. 1) [30], thus the correlations for three parties (the KS18 nonlocal correlations between Alice and Bob and the contextual correlations produced by sequentially measuring KS18 between Bob and Charlie) could be used to certify quantum transformations in a device-independent way. All these functionalities contribute to closing of the gap between general probabilistic theories (which refer to states, measurements, and transformations) and the device-independent framework (which refer only to the conditional probabilities of obtaining outputs from inputs) [69].

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[22] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevResearch.5.L012035 for concepts in KS contextuality (Appendix A), methods to obtain tight Bell inequalities (Appendix B), further details on our implementation of Gilbert's algorithm (Appendix C), the second step of our method (Appendix D), the Bell inequalities obtained (Appendix E), their optimality (Appendix F), why there are two optimal inequalities (Appendix G), device-independent applications of the KS18 and Yu-Oh correlations (Appendix H), and the proofs that two of the tight Bell operators have the same symmetries as the graph of compatibility of the corresponding SI-C set (Appendix I). The Supplemental Material includes Refs. [70–94].

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