Uncertainty Relations from State Polynomial Optimization

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Uncertainty relations are a fundamental feature of quantum mechanics. How can these relations be found systematically? Here, we develop a semidefinite programming hierarchy for additive uncertainty relations in the variances of noncommuting observables. Our hierarchy is built on the state polynomial optimization framework, also known as scalar extension. The hierarchy is complete in the sense that it converges to tight uncertainty relations. We improve upon upper bounds for all 1292 additive uncertainty relations on up to nine operators for which a tight bound is not known. The bounds are dimension-free and depend entirely on the algebraic relations among the operators. The techniques apply to a range of scenarios, including Pauli, Heisenberg-Weyl, and fermionic operators, and generalize to higher order moments and multiplicative uncertainty relations.

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Introduction.—Quantum mechanical particles exhibit a fundamental uncertainty relation between conjugate observables. Similar to probability distributions that are related by a Fourier transform, conjugate observables do not allow for simultaneous measurements with vanishing variances. This feature both enables as well as hinders certain applications of quantum technologies [1–6]. While commuting measurements can be jointly diagonalized, anticommuting observables are incompatible. This is taken advantage of in quantum error correction, where errors that anticommute with some stabilizer elements are detected by the change they induce in the respective error syndromes [5]. Also the security of quantum key distribution relies crucially on the fact that a basis change leads to an unavoidable uncertainty in measurement outcomes [6]. In particular, additive uncertainty relations find applications in spectroscopy and atomic clocks [7], and quantum metrology [8]. Considerable effort has been made to derive state-independent bounds [9,10].

To introduce our setting, consider a two-dimensional spin system with σ_x, σ_y, σ_z the Pauli matrices and denote $\langle\sigma_i\rangle_\varrho \coloneqq \mathrm{tr}(\varrho\sigma_i)$ the expectation value of σ_i on state ϱ. The set of a qubit density matrices is described by the Bloch ball, satisfying

$$\langle\sigma_x\rangle_\varrho^2 + \langle\sigma_y\rangle_\varrho^2 + \langle\sigma_z\rangle_\varrho^2 \leq 1. \tag{1}$$

A straightforward consequence of this constraint is an additive uncertainty relation of the form

$$\Delta^2\sigma_x + \Delta^2\sigma_y + \Delta^2\sigma_z \geq 2, \tag{2}$$

where $\Delta^2\sigma_i \coloneqq \langle\sigma_i^2\rangle_\varrho - \langle\sigma_i\rangle_\varrho^2$ and we used that $\sigma_i^2 = \mathbb{1}$. More generally, for a set of anticommuting operators the relation $\sum_{i=1}^n \langle\sigma_i\rangle^2 \leq 1$ holds. This follows from the decomposition $1 - \sum\langle\sigma_i\rangle_\varrho^2 = \langle(1 - \sum\sigma_i\langle\sigma_i\rangle_\varrho)^2\rangle \geq 0$ as sum of squares. A natural question is then what happens when some of the variables commute, while some others anticommute.

To answer this question we investigate the following quantity: given a family of Hermitian and unitary operators $\{A_i\}_{i=1}^n$ satisfying commutation relations of the form $A_iA_j = \pm A_jA_i$, define the quantity

$$\beta = \sup_\varrho \sum_{i=1}^n \langle A_i\rangle_\varrho^2. \tag{3}$$

Here, the maximization is over all states ϱ and bounded operators A_i on Hilbert spaces that support ϱ and the commutation relations between the A_i. Bounds on β have several applications in quantum information, including the characterization of entanglement [11], nonlocality [12], and measurement compatibility [13] and to estimate ground state energies [14]. Alternatively, Eq. (3) gives in the spirit of Eq. (2) tight additive uncertainty relation in the variances $\Delta^2A_i \coloneqq \langle A_i^2\rangle_\varrho - \langle A_i\rangle_\varrho^2$,

$$\sum_{i=1}^n \Delta^2A_i \geq n - \beta. \tag{4}$$

In a recent work [11], Gois *et al.* provided the upper bound $\beta \leq \vartheta(G)$. Here, $\vartheta(G)$ is the Lovász theta number of the observables anticommutativity graph. This graph encodes the observables' relations, with two vertices joined by an edge, if the corresponding observables anticommute; i.e., $i \sim j$ if $A_iA_j = -A_jA_i$ and $i \nsim j$ else. The related bound by Hastings and O'Donnell [15], $\langle\sum_{i=1}^n a_iA_i\rangle_\varrho^2 \leq \vartheta(G)$ for all $\|a\| \leq 1$, has been discovered in the context of optimizing fermionic Hamiltonians. In turn, β is lower bounded by the independence number α, which is the maximal number of disconnected vertices of G. The appearance of the Lovász theta number in this context is intriguing, as it

TABLE I. Tight uncertainty relations. The commutation relations of operators are encoded in a graph: two vertices are connected if the corresponding operators anticommute and disconnected otherwise. Our hierarchy [Eq. (15)] upper bounds $\beta = \sup_\varrho \sum_{i=1}^n \langle A_i \rangle_\varrho^2$ as $\beta \le \ldots \le \vartheta_2 \le \vartheta_1$, from which one obtains the additive uncertainty relation $\sum_{i=1}^n \Delta^2 A_i \ge n - \beta$. The independence number α is the size of the largest set of disconnected vertices and lower bounds β, while the Lovász number ϑ [Eq. (6)] provides an upper bound and coincides with the first level of our hierarchy. For the graphs shown above, the second level gives a tight uncertainty relation as $\alpha = \beta = \vartheta_2$, whereas ϑ_1 does not. The labeling is identical to that of Table IV.

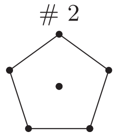
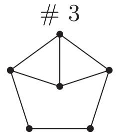
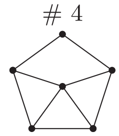
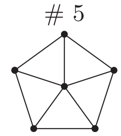
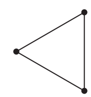
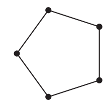
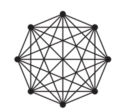
	# 2	# 3	# 4	# 5
				
ϑ_1	3.2361	2.2361	2.2361	2.2361
ϑ_2	3.0000	2.0000	2.0000	2.0000
α	3	2	2	2

TABLE II. Upper bounds ϑ_k for higher dimensional spin operators, obtained with an adaptation of Eq. (15) for commutation relations given by dth roots of unity, $A_i A_j = e^{2\pi i/d} A_j A_i$ when $i \sim j$. This requires complex moment matrices that can be evaluated through Eq. (22). Lower bounds (lb) are obtained from sampling Haar random states and evaluating them on Heisenberg-Weyl operators [Eq. (A13)]. Displacement operators [Eq. (A17)] give the same bounds.

		$d=2$	$d=3$	$d=5$
	ϑ_1	1.0000	1.0000	1.4906
	ϑ_2	1.0000	1.0000	1.4575
	lb	1.0000	1.0000	1.4500
	ϑ_1	2.2361	2.0000	2.3058
	ϑ_2	2.0000	2.0000	2.2001
	lb	2.0000	1.7770	1.2690
	ϑ_1	1.0000	2.0000	2.0000
	ϑ_2	1.0000	2.0000	2.0000
	lb	1.0000	2.0000	1.9940

has already been linked to nonlocality, contextuality, and quantum zero-error communication [16–19].

The aim of this Letter is to provide a semidefinite programming hierarchy that upper bounds Eq. (3) and improves upon the Lovász bound. The first level of our hierarchy coincides with the Lovász theta number, and thus with the result of Gois *et al.* Furthermore, if at any level of the hierarchy the upper bound coincides with α (c.f. Table I) or the rank loop condition is met, then the corresponding uncertainty relation in Eq. (4) is tight. Numerical tests show that already the second level of our hierarchy improves upon the previous best upper bounds for all 1292 nonisomorphic graphs with up to nine vertices for which β is unknown [20]. In particular, Table IV shows that the second and third levels often close the gap left by the Lovász theta number to a tight bound. We also introduce a second semidefinite programming hierarchy [Eq. (19)] that is complete and thus converges to β. With this we partially answer an open question by Xu *et al.* on how to obtain efficient upper bounds on β [14].

The central tool we use is state polynomial optimization by Klep *et al.* [21], also known as scalar extension [22,23], and which can be thought of as a variant of the noncommutative optimization framework by Navascués, Pironio, and Acín [24,25]. This makes the resulting bounds both independent of the local dimension and applicable to a wide range of situations. Different normalization conditions (e.g., projectors, unitaries, unipotents), commutation relations, and additive as well as multiplicative uncertainty relations in higher order moments can be treated. For example, Table II shows values of β for a set of Heisenberg-Weyl operators that satisfy commutation relations of the form $A_i A_j = \zeta_{ij} A_j A_i$ with ζ_{ij} a root of unity.

In this Letter, we will restrict the exposition to unitary operators and quadratic expressions as in Eq. (3). In what follows, upper case letters will refer to observables as in $\langle A \rangle_\varrho := \mathrm{tr}(\varrho A)$, while the lower case refers to letters a and words w in the state polynomial framework, whose evaluation on a state is referred to as $\langle a \rangle$ and $\langle w \rangle$.

Lovász bound.—We introduce the upper bound on β in Eq. (3) given by the Lovász theta number [11]. Let $\{A_1, \ldots, A_n\}$ be a collection of hermitian unitary operators that pairwise either commute or anticommute—for example, a collection of n-qubit Pauli operators. We encode the commutation relations $A_i A_j = \zeta_{ij} A_j A_i$ with ζ_{ij} in a graph G with adjacency matrix $\Gamma_{ij} = (1 - \zeta_{ij})/2$, where $\zeta_{ij} \in \{+1, -1\}$. In this way, every vertex represents an operator, with two vertices connected whenever the corresponding operators anticommute. The Lovász bound then constrains β as [11,15]

$$\beta \le \vartheta(G). \tag{5}$$

Here, $\vartheta(G)$ is the Lovász theta number of the graph G.

A for us convenient definition of $\vartheta(G)$ is through the optimal value of the following semidefinite program [26]:

$$\begin{aligned} \vartheta(G) &= \max_M \sum_{i=1}^n M_{ii} \\ \text{s.t. } M_{ii} &= a_i, \\ M_{ij} &= 0 \quad \text{if } \zeta_{ij} = -1, \\ \Delta &= \begin{pmatrix} 1 & a^T \\ a & M \end{pmatrix} \ge 0. \end{aligned} \tag{6}$$

To see how Eq. (6) gives an upper bound on Eq. (3), that is $\beta \leq \vartheta(G)$, consider the following relaxation: for any ϱ construct a moment matrix Γ indexed by the set $\{\mathbb{1}, \langle A_1^\dagger \rangle_\varrho A_1, \ldots, \langle A_n^\dagger \rangle_\varrho A_n\}$, where $\langle A_i \rangle_\varrho = \mathrm{tr}(\varrho A_i)$ and $A_0 = \mathbb{1}$,

$$\Gamma_{ij} = \mathrm{tr}(\varrho \langle A_i \rangle_\varrho \langle A_j^\dagger \rangle_\varrho A_i^\dagger A_j). \tag{7}$$

Such matrix Γ has the form

$$\begin{array}{c} \mathbb{1} \\ \langle A_1 \rangle_\varrho A_1^\dagger \\ \vdots \\ \langle A_n \rangle_\varrho A_n^\dagger \end{array} \overset{\begin{array}{cccc} \mathbb{1} & \langle A_1^\dagger \rangle_\varrho A_1 & \cdots & \langle A_n^\dagger \rangle_\varrho A_n \end{array}}{\begin{bmatrix} 1 & \Gamma_{01} & \cdots & \Gamma_{0n} \\ & \Gamma_{11} & \cdots & \Gamma_{1n} \\ & & \ddots & \vdots \\ & & & \Gamma_{nn} \end{bmatrix}}. \tag{8}$$

In particular, $\Gamma_{0i} = \Gamma_{ii} = \langle A_i \rangle_\varrho^2$ since $A_i^\dagger A_i = \mathbb{1}$, and Γ is positive semidefinite by construction. Also, we can set $\Gamma_{ij} = 0$ when $\zeta_{ij} = -1$, because if Γ is feasible, so is $(\Gamma + \Gamma^t)/2$ with the objective value unchanged. Note that these last three properties coincide with the constraints imposed on Δ in Eq. (6). However, a moment matrix Γ must additionally arise from some quantum state, and generally the set of matrices Δ can be larger than the set of matrices Γ arising from states. Consequently, the optimum of Eq. (6) upper bounds β and the Lovász bound holds, $\beta \leq \vartheta(G)$.

While this approach already gives tight upper bounds in several settings, the pentagon graph in Table II with $\beta = 2 < \sqrt{5} = \vartheta(G)$ shows that this Lovász bound is not tight in general. It turns out that a slight modification of the program in Eq. (6) can significantly strengthen the bounds. The key idea is to consider larger moment matrices, that incorporate additional commutativity constraints between products of operators.

A Lovász-type hierarchy.—To obtain stronger bounds, consider the set of moment matrices indexed by $\{\langle A_i^\dagger \rangle_\varrho \langle A_j^\dagger \rangle_\varrho A_i A_j\}_{0 \leq i < j \leq n}$ [27],

$$\Gamma_{ij,kl} = \mathrm{tr}(\varrho \langle A_i \rangle_\varrho \langle A_j \rangle_\varrho \langle A_k^\dagger \rangle_\varrho \langle A_l^\dagger \rangle_\varrho (A_i A_j)^\dagger A_k A_l). \tag{9}$$

These have the form

$$\begin{array}{c} \mathbb{1} \\ \vdots \\ \langle A_i \rangle_\varrho \langle A_j \rangle_\varrho (A_i A_j)^\dagger \\ \vdots \end{array} \overset{\begin{array}{cccc} \mathbb{1} & \cdots & \langle A_k^\dagger \rangle_\varrho \langle A_l^\dagger \rangle_\varrho A_k A_l & \cdots \end{array}}{\begin{bmatrix} 1 & \cdots & \Gamma_{00,kl} & \cdots \\ & \ddots & \vdots & \\ & & \Gamma_{ij,kl} & \cdots \\ & & & \ddots \end{bmatrix}}, \tag{10}$$

The submatrix $(\Gamma_{i0,j0})_{0 \leq i < j \leq n}$ coincides with Eq. (8), while the complete matrix satisfies additional second-order commutation relations,

$$\Gamma_{ij,kl} = \zeta_{ji} \Gamma_{\underline{ji},kl} = \zeta_{kl} \Gamma_{ij,\underline{lk}} = \zeta_{ik} \Gamma_{\underline{kj},\underline{il}}. \tag{11}$$

Again, Γ is positive semidefinite.

Thus in analogy to Eq. (6), we formulate the relaxation

$$\begin{aligned} \vartheta_2(G) = \max_M & \sum_{i=1}^n M_{i0,i0} \\ \text{s.t. } & M_{ij,kl} = \zeta_{ji} M_{ji,kl}, \\ & M_{ij,kl} = \zeta_{kl} M_{ij,lk}, \\ & M_{ij,kl} = \zeta_{ik} M_{kj,il}, \\ & M_{ii,kl} = M_{0i,kl}, \\ & M \geq 0. \end{aligned} \tag{12}$$

As in the previous section, we can restrict to real matrices: if M is feasible, then so is $(M + M^t)/2$ with unchanged objective value. Thus we can set $M_{ij,kl} = 0$ if $(A_i A_j)^\dagger A_k A_l = -(A_k A_l)^\dagger A_i A_j$. Later on, we cover the general case with non-Hermitian operators and complex phases [Eq. (19)], which requires complex matrices.

In analogy to the argument made for the Lovász bound, any Γ matrix arising from a state also satisfies the constraints imposed on the matrix M in Eq. (12). Thus the set of valid moment matrices Γ is contained in the set of feasible matrices M. Consequently, $\beta \leq \vartheta_2(G)$. Additionally, as the submatrix $(M_{i0,j0})_{i,j=0}^n$ coincides with Δ of Eq. (6), we have the strengthening

$$\beta \leq \vartheta_2(G) \leq \vartheta(G). \tag{13}$$

For the pentagon graph in Table II, this enlarged program already yields a tight bound on $\beta = 2 = \vartheta_2(G)$. For the remaining graphs with five vertices the Lovász number equals the independence number, and thus $\vartheta_2(G)$ is tight for all graphs with up to five vertices.

The argument above easily generalizes to larger indexing sequences that incorporate commutation relations between products of up to k operators. Denote $\vec{i} = (i_1, \ldots, i_k)$, a moment matrix Γ indexed by $\{\langle A_{i_1}^\dagger \rangle_\varrho \ldots \langle A_{i_k}^\dagger \rangle_\varrho A_{i_1} \ldots A_{i_k}\}_{i_1, \ldots, i_k = 0}^n$ where all nonzero indices are pairwise distinct and ordered increasingly. This has entries

$$\begin{aligned} \Gamma_{\vec{i},\vec{j}} = & \langle A_{i_1} \rangle_\varrho \ldots \langle A_{i_k} \rangle_\varrho \langle A_{j_1}^\dagger \rangle_\varrho \ldots \langle A_{j_k}^\dagger \rangle_\varrho \\ & \times (\langle A_{i_1} \ldots A_{i_k})^\dagger A_{j_1} \ldots A_{j_k} \rangle_\varrho \end{aligned} \tag{14}$$

and satisfies the semidefinite program

$$\begin{aligned} \vartheta_k(G) = \max_M & \sum_{i=1}^n M_{0\ldots 0i, 0\ldots 0i} \\ \text{s.t. } & M_{\pi(a,b)(\vec{i},\vec{j})} = \xi_{ab} M_{\vec{i},\vec{j}}, \\ & M_{ii\ldots i_k, \vec{j}} = M_{0i\ldots i_k, \vec{j}}, \\ & M \geq 0. \end{aligned} \tag{15}$$

Here, $\pi(a,b)$ is the transposition exchanging the ath and bth elements in the joint sequence $(i_k,\ldots,i_1,j_1,\ldots,j_k)$ (note the reversed indexing in the index i arising from the dagger in the moment matrix) and

$$\xi_{ab} = \prod_{a<c\le b} \zeta_{ac}\zeta_{cb} \tag{16}$$

is the factor that appears from the exchange.

By construction, Eq. (15) defines a hierarchy of upper bounds $\vartheta_k(G)$:

$$\beta(G) \le \ldots \le \vartheta_k(G) \le \ldots \le \vartheta_1(G) = \vartheta(G). \tag{17}$$

We show in the next section that the relaxations ϑ_k in Eq. (15), in particular ϑ in Eq. (6), can be enlarged to a complete hierarchy of semidefinite programs converging to the optimal value of Eq. (3).

A complete hierarchy.—We now present a complete hierarchy that converges to β. Let ζ be a matrix encoding the commutation relations between a collection of operators $\{A_1,\ldots,A_n\}$. The upper bound β in Eq. (3) can be formulated as the following optimization problem over expectations $\langle\cdot\rangle_\varrho$:

$$\begin{aligned} &\sup_\varrho \sum_{i=1}^n |\langle A_i\rangle_\varrho|^2 \\ &\text{s.t. } A_i^\dagger A_i = A_i A_i^\dagger = 1, \\ &\quad A_i A_j = \zeta_{ij} A_j A_i, \\ &\quad \langle \mathbb{1}\rangle_\varrho = 1. \end{aligned} \tag{18}$$

We now show how to tackle this problem with a variant of noncommutative polynomial optimization [24], allowing for nonlinear expressions in the expectations, known as state polynomial optimization [21] or scalar extension [28].

To solve this type of optimization problem, consider words (or noncommutative monomials) $w = a_{j_1}\cdots a_{j_p}$ built from letters $\{a_i\}_{i=1}^n$ and expectation value of words denoted by $\langle w\rangle = \langle a_{j_1}\cdots a_{j_p}\rangle$. The most general monomials in words and expectations are then of the form $w = w_0\langle w_1\rangle\cdots\langle w_m\rangle$. Such formal state monomials can be added and multiplied to form state polynomials. The involution of a word is defined by $(a_1\ldots a_n)^* = a_n^*\ldots a_1^*$, which plays the role of the adjoint of an operator in the formal setting. In particular, $a_i^* = a_i$ when the operators are required to be Hermitian. Also, expectations behave as scalars, so that $v\langle w\rangle = \langle w\rangle v$ for all v, w. Finally, $\langle v\langle w\rangle\rangle = \langle\langle v\rangle\langle w\rangle\rangle = \langle v\rangle\langle w\rangle$ and $(v\langle w\rangle)^* = v^*\langle w\rangle^* = \langle w\rangle^* v^*$, while e is the identity (or empty) word satisfying $we = w = ew$ for all words w.

For our problem, one additionally imposes the constraints $a_i a_j = \zeta_{ij} a_j a_i$ arising from the commutation relations $A_i A_j = \zeta_{ij} A_j A_i$. Likewise, the constraint $A_i^\dagger A_i = A_i A_i^\dagger = \mathbb{1}$ gives rise to $a_i^* a_i = a_i a_i^* = e$. For Pauli matrices, this reduces all monomials to square-free monomials.

Now consider a moment matrix M_ℓ, indexed by all state monomials of degree at most ℓ, whose entries are $M_\ell(v,w) = \langle v^* w\rangle$. Then, the optimal solution of Eq. (18) is approximated from above with the following hierarchy of semidefinite programs with $\ell\in\mathbb{N}$ [[21], Lemma 6.5]:

$$\begin{aligned} &\nu_\ell(\zeta) = \max \sum_{i=1}^n |\langle a_i\rangle|^2 \\ &\text{s.t. } \langle \mathrm{id}\rangle = 1, \\ &M_\ell(v,w) = M_\ell(x,y) \quad \text{when} \quad \langle v^* w\rangle = \langle x^* y\rangle, \\ &M_\ell \ge 0, \end{aligned} \tag{19}$$

where one imposes on the entries M_ℓ all relations arising from $a_i a_j = \zeta_{ij} a_j a_i$ and $a^* a = a a^* = e$. By increasing the degree ℓ, these relaxations converge to the optimal solution of Eq. (3) [[21], Theorem 5.5 and Proposition 6.7]:

$$\lim_{\ell\to\infty} \nu_\ell(\zeta) = \beta. \tag{20}$$

For this result to hold, it is necessary that the optimization is over a bounded set of operators. The technical condition is that the set is Archimedean, that is, there exists a constant $C > 0$, such that $\sum_{i=1}^n a_i a_i^* \le C$. In our problem this is satisfied with $C = n$. Additionally, when the rank loop condition is met, that is $\mathrm{rank}(M_\ell) = \mathrm{rank}(M_{\ell+1})$ (this is called a flat extension), then the optimum has been reached [[21], Proposition 6.10].

It can now be seen that $\vartheta_k(G)$ of Eq. (15) arises from the state polynomial optimization framework [Eq. (19)] where one considers only state monomials of the form

$$\{\langle a_{i_1}^*\rangle\cdots\langle a_{i_k}^*\rangle a_{i_1}\cdots a_{i_k}\}_{i_1,\ldots,i_k=0}^n, \tag{21}$$

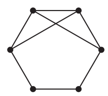
with all nonzero indices pairwise distinct.

Non-Hermitian operators.—Note that both the complete and relaxed hierarchies can easily deal with operators that neither commute nor anticommute, but for which there is a complex phase $\zeta_{ij}\in\mathbb{C}$. Then for every letter a we define two new symbols to denote its real $\Re w$ and imaginary $\Im w$ part. Additionally, for each word w impose the constraints $\Re w = \Re w^*$ and $\Im w = -\Im w^*$. The positive semidefinite constraint on the complex moment matrix $M_\ell = \Re M_\ell + i\Im M_\ell \ge 0$ is equivalent to

$$\begin{pmatrix} \Re M_\ell & -\Im M_\ell \\ \Im M_\ell & \Re M_\ell \end{pmatrix} \ge 0. \tag{22}$$

Table II shows the first two levels of the hierarchy of Lovász relaxations for the Heisenberg-Weyl operators computed through the complex to real mapping of Eq. (22). These operators are not Hermitian in dimensions d greater than two, and we use weighted graphs to specify their commutation relations where ζ_{ij} is a dth root of unity. Note that the cost of solving the problem in Eq. (19) does

TABLE III. Cutting planes in graph #3. Left: ϑ_k of Eq. (15). Right: ϑ_k strengthened with two intertwined 5-holes inequalities [Eq. (23)].



ϑ_1	2.2361	2.2356
ϑ_2	2.0000	2.0000
α	2	

not increase with d but only with the number of operators and the level of the hierarchy k.

Cutting planes.—The Lovász bound in Eq. (6) can be strengthened with additional constraints—for instance with so-called odd-hole inequalities [26]. Let G be the anticommutation graph of some Hermitian operators, and let H be a subset of vertices of G inducing a cycle (i.e., a hole). Then

$$\sum_{i\in H}\langle A_i\rangle_\varrho^2 \le \left\lfloor\frac{|H|}{2}\right\rfloor. \tag{23}$$

This constraint acts as a half-plane in the semidefinite program, and can strengthen the Lovász bound for odd $|H|$. For graphs with up to seven vertices with nonoverlapping holes, these additional constraints are enough to tighten the bound for β. However, these are not enough when the holes are intertwined as in Table III (#3 in Table IV). More generally, one can impose constraints that arise from higher levels in the hierarchy [Eq. (19)] on selected subgraphs.

Conclusions.—We presented in Eq. (19) a complete semidefinite programming hierarchy converging to tight uncertainty relations. The reduced formulation of this hierarchy in Eq. (15) can be seen as a natural generalization of the Lovász bound [11]. Interestingly, the second level of this reduced hierarchy already provides tight bounds on β for all graphs with no more than six vertices. This answers an open question by Xu *et al.* on how to efficiently bound β [14]. Additionally, our hierarchy applies to a wide range of scenarios, including the n-qubit Pauli group, generalized Pauli operators for higher-dimensional systems, Clifford algebras, and fermionic operators. It also applies to higher order moments and multiplicative uncertainty relations. Several questions remain. (1) Can a similar approach be derived for entropic uncertainty relations [29–34]? (2) Can uncertainty relations for Gell-Mann matrices be found that make use of the structure constants of SU(3), in analogy to the Lovász bound? (3) Is the hierarchy of relaxations $\vartheta_k(G)$ in Eq. (15) complete, in the sense that it converges to β? (4) Can sparsity [35] or symmetry [36–40] reductions boost efficiency of the semidefinite programs? (5) Which hyperplane constraints improve the Lovász bound most without incurring a too high computational overhead [26]? How do these constraints differ from the classical case? (6) The weight enumerators describing quantum error correcting codes can be expressed as sums over $|\langle A_i\rangle|^2$. Can also here a Lovász bound be established to upper bound the size of a quantum code? (7) Can structure theorems for quasi-Clifford algebras or quantum tori [41,42] help to derive algebraic bounds? Are there any significant changes with respect to the choice of the matrix basis [43]—for example, when considering nice error bases [44]?

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Appendix: Further applications.—Already for Hermitian operators, Eq. (3) finds applications in the characterization of entanglement and nonlocality. For example, Eq. (1) gives the entanglement witness [11]

$$W = \mathbb{1}\otimes\mathbb{1} - \sigma_x\otimes\sigma_x - \sigma_y\otimes\sigma_y + \sigma_z\otimes\sigma_z. \tag{A1}$$

It holds that $\langle W\rangle_\varrho \ge 0$ for all separable states ϱ, whereas a joint eigenstate of $\sigma_x\otimes\sigma_x$, $\sigma_y\otimes\sigma_y$, and $\sigma_z\otimes\sigma_z$ achieves a value $\langle W\rangle_\varrho = -2$.

Similar constraints involving Pauli strings bound the quantum value of Bell inequalities [45] and Bell monogamy [12]. For instance, let $\mathcal{L}$ be a Bell inequality with two measurements with two outcomes between two parties. Normalizing the value over classical correlations as $\mathcal{L}\le 1$, the optimal quantum value is obtained by the value in Eq. (3) for the following Pauli strings

$$\mathcal{L}^2 \le \langle\sigma_x\otimes\sigma_x\rangle^2 + \langle\sigma_x\otimes\sigma_y\rangle^2 + \langle\sigma_y\otimes\sigma_x\rangle^2 + \langle\sigma_y\otimes\sigma_y\rangle^2 \le 2. \tag{A2}$$

This gives the Tsirelson's bound for the Clauser-Horne-Shimony-Holt inequality. More generally, upper bounds on Eq. (3) for Pauli strings yield upper bounds for the quantum value of Bell inequalities and Bell monogamy involving only dichotomic measurements [12,45]. It is an interesting question whether the bound in Eq. (A2) extends to measurements with more than two outcomes.

As noticed in Ref. [14], Eq. (3) also bounds the ground state energy of the Hamiltonian $H = \sum_i^n A_i$, since $\langle H\rangle^2 \le n\sum_i^n\langle A_i\rangle^2$. These bounds are determined by the algebraic relations between the terms and thus are independent of the physical dimension.

The Lovász theta number: A *graph*$G = (V, E)$ consists of a set V of *vertices* and a set $E\subset V\times V$ of *edges* between them. Two vertices $u, v\in V$ are connected ($u\sim v$)

when $(u,v)\in E$, and disconnected or *independent* otherwise. The *complement* of G is $\bar{G}=(V,\bar{E})$, where $(u,v)\in\bar{E}$ if and only if $(u,v)\notin E$.

The *independence number* $\alpha(G)$ is the maximum number of pairwise independent vertices of G. The *chromatic number* $\chi(G)$ is the minimum number of different colors needed to assign to the vertices of G, such that no connected vertices share the same color. These quantities, also called *graph invariants*, encode key combinatorial properties of G and are NP-complete [46].

However, some graph invariants capture properties of the graph that are easier to compute. Of particular interest is the *Lovász number* $\vartheta(G)$, which is sandwiched by the two quantities described above [47],

$$\alpha(G)\leq\vartheta(G)\leq\chi(\bar{G}). \tag{A3}$$

It can be computed in polynomial time since it can be defined through a semidefinite program [48],

$$\begin{aligned}\vartheta(G)=&\max_{M}\sum_{i,j=1}^{n}M_{ij}\\ \text{s.t.}\ &\mathrm{tr}(M)=1\\ &M_{ij}=0\quad\text{if } i\sim j\\ &M\geq 0.\end{aligned} \tag{A4}$$

Equivalent definitions for $\vartheta(G)$ are [26]

$$\begin{aligned}\vartheta(G)=&\max_{M}\sum_{i=1}^{n}M_{ii}\\ \text{s.t.}\ &M_{ii}=a_i\\ &M_{ij}=0\quad\text{if } i\sim j\\ &\Delta=\begin{pmatrix}1 & a^T\\ a & M\end{pmatrix}\geq 0,\end{aligned} \tag{A5}$$

and [47]

$$\begin{aligned}\vartheta(G)=&\max_{M}\lambda_{\max}(M)\\ \text{s.t.}\ &M_{ii}=1\\ &M_{ij}=0\quad\text{if } i\sim j\\ &M\geq 0,\end{aligned} \tag{A6}$$

where $\lambda_{\max}(M)$ denotes the maximum eigenvalue of M.

Given a collection of Hermitian unitary operators $A_1,\ldots,A_n$ that mutually either commute or anticommute, define the *anticommutativity graph* G on vertices $\{1,\ldots,n\}$ where $i\sim j$ if $A_iA_j=-A_jA_i$. The quantity

$$\beta=\sup_{\varrho}\sum_{i=1}^{n}\langle A_i\rangle_{\varrho}^2 \tag{A7}$$

is then a graph invariant that is defined solely through the commutation relations encoded in G. Commuting operators can be jointly diagonalized; thus, it is clear that $\alpha(G)\leq\beta(G)$: a joint eigenstate simultaneously achieves the value $\langle A_i\rangle_{\varrho}^2=1$ for each term in an independent set. On the other hand, Ref. [11] showed that $\beta(G)\leq\vartheta(G)$ by using the definition in Eq. (A6).

As an example, take the following five two-qubit Pauli observables

$$\sigma_x\otimes\sigma_x,\quad \sigma_x\otimes\sigma_y,\quad \mathrm{id}\otimes\sigma_x,\quad \sigma_y\otimes\sigma_z,\quad \sigma_y\otimes\sigma_x. \tag{A8}$$

Their anticommutativity graph is the pentagon $G=C_5$ shown in Table IV. The second level of the hierarchy improves on the Lovász bound, closing the gap with the independence number and thus giving the tight bound

$$2=\alpha(C_5)=\beta(C_5)=\vartheta_2(C_5)<\vartheta_1(C_5)=\sqrt{5}. \tag{A9}$$

Comparison with previous work: Upper bounds in Ref. [14] are obtained fixing a representation of the operators $(A_1,\ldots,A_n)$ as Pauli strings in dimension 2^N, through the separability problem

$$\begin{aligned}&\max_{\sigma}\sum_{i=1}^{n}\langle A_i\otimes A_i\rangle_{\sigma}\\ &\text{s.t.}\ \sigma\in\mathrm{SEP}.\end{aligned} \tag{A10}$$

Here, the maximization runs over separable states on $\mathbb{C}^{2\otimes N}\otimes\mathbb{C}^{2\otimes N}$. This problem can be outer-approximated with semidefinite programs based on symmetric extension. Level $k\in\mathbb{N}$ of this hierarchy corresponds to

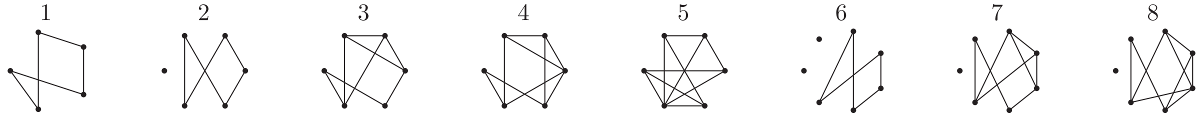
$$\begin{aligned}&\max_{\sigma}\sum_{i=1}^{n}\langle A_i\otimes A_i\rangle_{\sigma}\\ &\text{s.t.}\ \sigma\in\mathrm{Sym}_k.\end{aligned} \tag{A11}$$

Here, the maximization runs over all states $\sigma=\sigma_{AB_1\ldots B_k}$ on $(\mathbb{C}^2)^{\otimes N}\otimes(\mathbb{C}^2)^{\otimes[N(1+k)]}$ that are invariant under exchange of the subsystems $B_1,\ldots,B_k$, with positive partial transpose across all bipartitions. The dimension of this hierarchy grows as $2^{N(2+k)}$, which renders the relaxations intractable quickly.

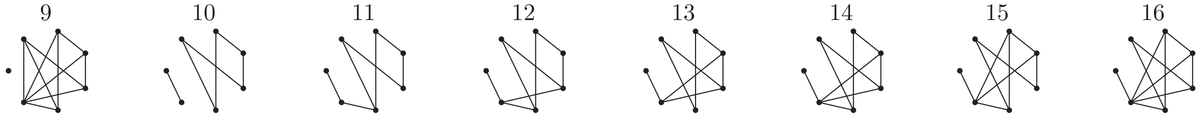
For instance, take the graph $G=\bar{C}_7$, the complement of the cycle with seven vertices. These operators can be represented with Pauli strings of $N=3$ qubits. The first extension has size $2^9=512$, which is already quite large for a desktop computer to solve.

Our approach based on state polynomial optimization [Eq. (18)] does not fix a representation, and is thus dimension-independent. The size of the relaxations is given by the size of the indexing sequence for the moment matrix in Eq. (19), which allows a finer control and flexibility in the size. In particular, our hierarchy $\vartheta_k(G)$ in Eq. (15) requires for a graph G with n vertices to solve SDPs of size $1+n$ for $\vartheta_1(G)$ [Eq. (6)], size $1+n(n+1)/2$ for $\vartheta_2(G)$ [Eq. (12)], and size 2^n+1 for $\vartheta_n(G)$. For a graph G with

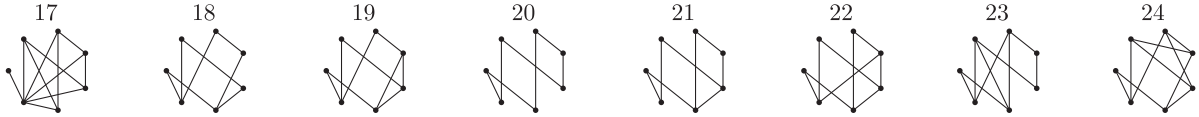
TABLE IV. Hierarchy of upper bounds for all nonisomorphic graphs up to seven vertices for which $\beta < \vartheta_1$. Our hierarchy ϑ_k in Eq. (15) improves on the bounds given by the Lovász number ϑ_1 in Eq. (6) and closes the gap for all but seven graphs: 33, 35, 37, 38, 39, 41, and 43.



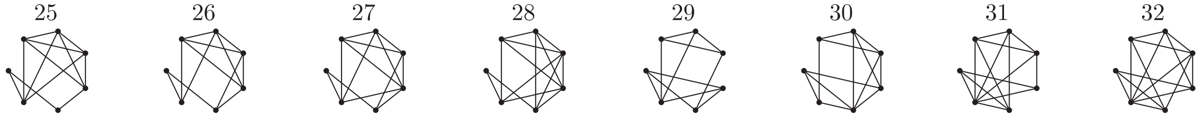
	1	2	3	4	5	6	7	8
ϑ_1	2.2361	3.2361	2.2361	2.2361	2.2361	4.2361	3.2361	3.2361
ϑ_2	2.0000	3.0000	2.0000	2.0000	2.0000	4.0000	3.0000	3.0000
α	2	3	2	2	2	4	3	3



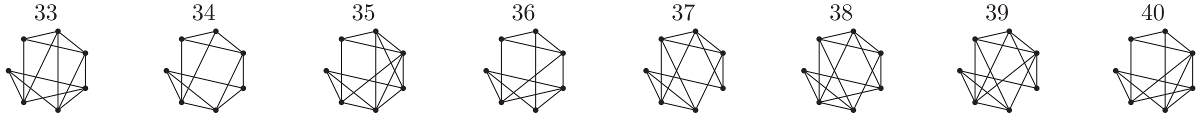
	9	10	11	12	13	14	15	16
ϑ_1	3.2361	3.2361	3.2361	3.2361	3.2361	3.2361	3.2361	3.2361
ϑ_2	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000
α	3	3	3	3	3	3	3	3



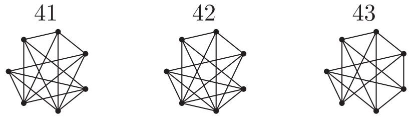
	17	18	19	20	21	22	23	24
ϑ_1	3.2361	3.1966	3.0642	3.3177	3.2361	3.1966	3.2361	3.1966
ϑ_2	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000
α	3	3	3	3	3	3	3	3



	25	26	27	28	29	30	31	32
ϑ_1	2.2361	2.2361	2.2361	2.2361	2.2361	2.2361	2.2361	2.2361
ϑ_2	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000
α	2	2	2	2	2	2	2	2



	33	34	35	36	37	38	39	40
ϑ_1	2.2361	2.2361	2.2361	2.2361	2.2361	2.2361	2.2361	2.2361
ϑ_2	2.0363	2.0056	2.0085	2.0033	2.0249	2.0392	2.0121	2.0024
ϑ_3	2.0067	2.0004	2.0017	2.0000	2.0047	2.0052	2.0006	2.0000
ϑ_7	2.0013	2.0000	2.0003	2.0000	2.0014	2.0011	2.0002	2.0000
α	2	2	2	2	2	2	2	2



	41	42	43
ϑ_1	2.2361	2.2361	2.1099
ϑ_2	2.0910	2.0000	2.0950
ϑ_3	2.0076	2.0000	2.0938
ϑ_7	2.0024	2.0000	2.0938
α	2	2	2

seven vertices such as $\bar{C}_7$, $\vartheta_7(G)$ has size $2^7 = 128$, which can easily be solved on a desktop computer.

In the approach by Ref. [14] the size of the resulting SDPs depends on whether the commutation relations can be represented on a small number of qubits, while it only depends on the number of observables for our hierarchies. However, with the symmetric extension approach one in principle is able to give approximation guarantees through the quantum de Finetti theorem [49].

Small graphs: Table IV shows all 43 nonisomorphic graphs with up to seven vertices for which $\beta < \vartheta_1$. Strengthening ϑ_1 with odd-hole inequalities as in Eq. (23), we obtain tight bounds on β for 18 graphs by matching the upper bounds with the independence number. For all but 10 of these graphs it holds that $\beta = \vartheta_2$, and $\beta = \vartheta_3$ holds for all but seven graphs.

Our hierarchy also improves on the best known upper bounds for all 36 nonisomorphic graphs with eight vertices and all 1256 nonisomorphic graphs with nine vertices for which the value of β is unknown [20]. Already our second level [Eq. (12)] gives tight bounds $\beta(G) = \vartheta_2(G)$ for four of those graphs, up to numerical precision.

Non-Hermitian operators:

Heisenberg-Weyl basis. The Heisenberg-Weyl operators can be seen as a generalization of the Pauli matrices. They play a central role in the description of d-dimensional quantum spin systems [43] and in the construction of nonbinary quantum codes [50]. On the space $\mathbb{C}^d$ define the operators X and Z through [51]

$$X|j\rangle = |j+1\rangle, \qquad Z|j\rangle = \omega^j |j\rangle, \tag{A12}$$

where $\omega = \exp(2\pi i/d)$ is the principal root of unity and the addition is taken modulo d. These operators are related by the quantum Fourier transform in dimension d. The collection of operators

$$\sigma(k,l)|i\rangle = X^k Z^l |i\rangle = \omega^{il}|i+k\rangle, \tag{A13}$$

forms the Heisenberg-Weyl basis for the space of complex $d \times d$ matrices. These satisfy the commutativity relations

$$\sigma(k,l)\sigma(m,n) = \omega^{lm-kn}\sigma(m,n)\sigma(k,l). \tag{A14}$$

Their adjoints are given by

$$\sigma(k,l)^\dagger = \omega^{kl}\sigma(d-k, d-l), \tag{A15}$$

and they form an orthogonal basis

$$\mathrm{tr}[\sigma(k,l)^\dagger \sigma(m,n)] = \delta_{km}\delta_{ln} d. \tag{A16}$$

Displacement basis. Introducing a phase [51],

$$D(k,l) = \omega^{kl/2}\sigma(k,l), \tag{A17}$$

the adjoint operators are given by

$$D(k,l)^\dagger = (-1)^{k+l+d} D(d-k, d-l). \tag{A18}$$

These are called displacement operators, and the algebra they generate is isomorphic to the one generated by Heisenberg-Weyl operators. Thus, the bounds for the non-Hermitian version of Eq. (18) coincide for both choices of generators (c.f. Table II).

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