Bounding the Joint Numerical Range of Pauli Strings by Graph Parameters

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The relations among a given set of observables on a quantum system are effectively captured by their so-called joint numerical range, which is the set of tuples of jointly attainable expectation values. Here we explore geometric properties of this construct for Pauli strings, whose pairwise commutation and anti-commutation relations determine a graph G. We investigate the connection between the parameters of this graph and the structure of minimal ellipsoids encompassing the joint numerical range, and we develop this approach in different directions. As a consequence, we find counterexamples to a conjecture by de Gois *et al.* [Phys. Rev. A 107, 062211 (2023)], and answer an open question raised by Hastings and O'Donnell [*STOC 2022: Proceedings of the 54th Annual ACM SIGACT Symposium on Theory of Computing*, pp. 776–789], which implies a new graph parameter that we call "$\beta(G)$." Furthermore, we provide new insights into the perennial problem of estimating the ground-state energy of a many-body Hamiltonian. Our methods give lower bounds on the ground-state energy, which are typically hard to come by, and might therefore be useful in a variety of related fields.

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I. INTRODUCTION

Pauli strings, i.e., tensor products of families of Pauli operators acting on multiple qubits, are undeniably among the most essential and omnipresent objects in the field of quantum information theory. In addition to their role as unitary transformations, they commonly also serve as fundamental building blocks for constructing observables. Examples of such constructed observables are widespread, ranging from virtually every Hamiltonian that is considered in the field of quantum computing [1–5] to typical measurements in quantum communication protocols [6–9] and to the rich theory of spin systems in condensed-matter physics [10–16].

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A pivotal object of investigation in this context is the set of jointly attainable expectation values. For a given set of n Pauli strings $\mathcal{S} = \{S_1, \ldots, S_n\}$ acting on the Hilbert space $\mathcal{H}$, we will consider

$$J(\mathcal{S}) = \left\{ \left(\langle S_1 \rangle_\rho, \ldots, \langle S_n \rangle_\rho \right) | \rho \in \mathcal{D}(\mathcal{H}) \right\}, \qquad (1)$$

which is a compact convex subset of $\mathbb{R}^n$ (see Fig. 1 for examples); here and subsequently, $\mathcal{D}(\mathcal{H})$ denotes the set of all states on the Hilbert space $\mathcal{H}$, i.e., density matrices, which are positive semidefinite and of unit trace.

For a general sequence $\mathcal{S}$ of observables, $J(\mathcal{S})$ in Eq. (1) is commonly referred to as the (convex) joint numerical range [17–23], or convex support. For special sets of observables, this set may, however, have more specific names, depending on the context. The most prominent example of this surely is the well-known Bloch ball (aka Bloch sphere), which can be understood as the joint numerical range of the three Pauli operators acting on a single qubit, i.e., $\mathcal{S} = \{X, Y, Z\}$.

For a more complex set of strings, the geometry of $J(\mathcal{S})$ is no longer necessarily captured by a sphere. Nevertheless, one can still ask for the smallest radius of a sphere

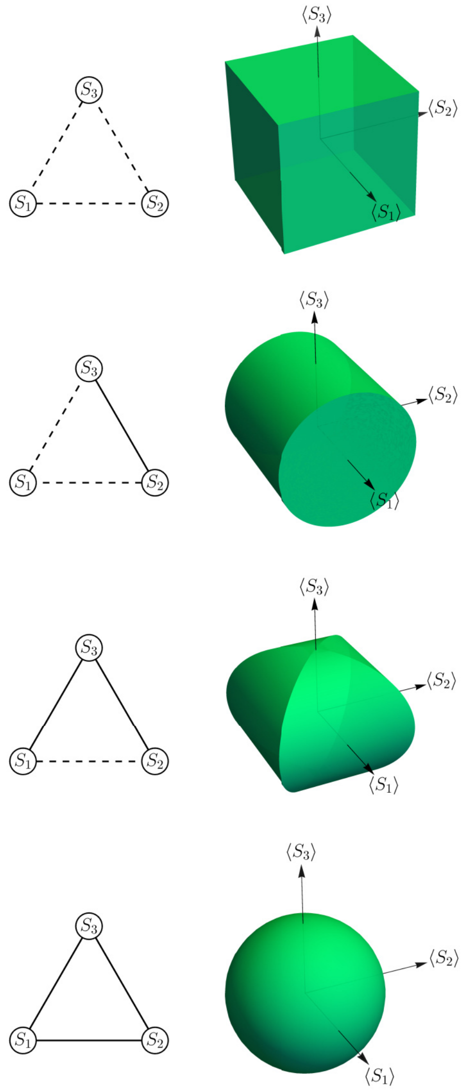

FIG. 1. Joint numerical ranges of three Pauli strings whose commutation and anticommutation relations are represented by the four possible graphs of three vertices. The real lines represent the anticommutation relations and the dashed lines stand for commutation relations.

or more generally an ellipsoid encompassing it. From a purely geometric perspective, this is the question tackled in the present work.

The joint numerical range geometrically encodes much relevant information about the interplay between observables and quantum states. Most strikingly, Hamiltonians that can be written as linear combinations of elements in $\mathcal{S}$ can be directly understood as linear functionals acting on $J(\mathcal{S})$. Correspondingly, the quest of finding ground-state energies and properties of states attaining them can be cast as the characterization of tangential hyperplanes on $J(\mathcal{S})$. Moreover, upper and lower bounds to ground-state energies correspond to inner and outer approximations of $J(\mathcal{S})$.

This insight, however, directly reveals that the precise characterization of the joint numerical range can, even for simple objects such as Pauli strings, be an intrinsically hard problem, i.e., at least as hard as solving ground-state problems on multiple qubits. This clearly justifies the demand for practical approximation techniques.

For the ground-state energy problem itself, there is a large toolbox of known methods. Most of them provide lower bounds (inner bounds on $J(\mathcal{S})$) by restricting the optimization to a suitable variational class of states. Prominent examples to be mentioned here include classical methods building on matrix product states [16,24,25], as well as implementations on quantum computers where algorithms such as the quantum approximate optimization algorithm [26–28] or the variational quantum eigensolver [29,30] are very popular.

Methods for outer approximations, on the other hand, are rare. In contrast to variational methods, the handling of global structures is needed, which is typically much harder to achieve. Nevertheless, they can be of central importance. On one hand, outer bounds give complements for inner approximations and, by this, an interval for the overall accuracy of an approximation attempt. On the other, the existence of a bound that cannot be surpassed by any quantum state, also including those that are not in a variational class, can be critical in applications such as cryptography or entanglement detection.

Notable examples of outer approximations can be found in Refs. [31–33]. Here, the ansatz is to exploit the algebraic structure of the problem for setting up hierarchies of noncommutative polynomial relaxations [34,35]. Even though the scope of these methods is to solve a particular ground-state problem, the feasible set of such a relaxation, sometimes called the "relaxation of the quantum set," can be seen as an outer approximation to the joint numerical range $J(\mathcal{S})$. On the theoretical side, those methods usually come with a convergence guarantee. In practice, however, they tend to show a very bad scaling behavior and typically saturate any practical limit of computational resources very quickly.

In the present work, we move towards a (semi)analytical understanding of $J(\mathcal{S})$. For an m-dimensional ellipsoid $\mathcal{E}_r(w)$ with principal axes of length $r/\sqrt{w_i}$, where $w = (w_1, \dots, w_m)$ is a positive weight vector, we ask for the smallest $r \geq 0$ such that

$$J(\mathcal{S}) \subseteq \mathcal{E}_r(w) \tag{2}$$

holds. Such a minimal ellipsoid, or at least an upper bound on r, then allows us to compute bounds on ground-state energies analytically. This is especially interesting when we deal with high-dimensional objects, i.e., for long Pauli strings where the Hilbert space dimension scales exponentially. We have to clarify that the deployment of a new numerical toolbox is, however, not within the scope of the present work, and we leave this for a future investigation. Here our main interest is to develop the foundations for a comprehensive understanding of the structures presented.

Finding a valid r, the optimal value of which we refer to as the "(generalized) radius," corresponds to the nonlinear optimization

$$r^2 \geq \sup_{\rho} \sum w_i \langle S_i \rangle_{\rho}^2. \tag{3}$$

Formally, this can be seen as an instance of so-called spectrahedral inclusion problems [36,37], for which there are unfortunately no out-of-the-box solutions. Hence, much of the particular structure of the present problem has to be leveraged in the solution.

The structure of minimal ellipsoids, as well as the structure of $J(\mathcal{S})$ itself (see Fig. 1), is closely related to a graph G that encodes the commutation and anticommutation relations within the strings of a set $\mathcal{S}$. This graph is also known as a "frustration graph" [11,12], an "anticommutation graph" [38], or an "anticompatibility graph" [39] in the literature. It can be shown [31,40] (see Proposition 2) that the minimal radius of an ellipsoid is lower-bounded by the weighted independence number of G and is upper-bounded by its weighted Lovász number. While being efficiently computable, the Lovász number as an upper bound is known to be generally not tight [31,40]. The tightness of the lower bound was, however, outstanding. For the spheroidal case $w = (1, 1, \ldots)$, it was conjectured [40], and extensively discussed during the coffee breaks at some workshops, that the independence number of G describes the minimal radius. We show by an explicit example that this conjecture is false.

As a consequence, we introduce the minimal radius of an ellipsoid as a new graph parameter $\beta(G, w)$ and embark on its exploration. We develop a number of equivalent formulations of it, we show that it is monotonic nonincreasing when passing to an induced subgraph, we show that it is multiplicative under the so-called lexicographic product, and we show several other properties. We calculate it for cyclic graphs C_n and develop numerical tools to evaluate it for the complements of odd cycles $\overline{C}_{2n+1}$, supporting our conjecture that $\beta(\overline{C}_{2n+1}) > 2$ for all $n \geq 3$. Lastly, we also elaborate on the connection of our results to the quest for uncertainty relations between Pauli strings as their structure also depends directly on the structure of minimal ellipsoids [40,41].

Our results connect multiple topics in quantum theory, graph theory, and algebra analysis, and so we believe that they might provide new insights in those fields as well.

II. OPERATOR REPRESENTATIONS OF GRAPHS, GRAPH PARAMETERS, AND MAIN RESULTS

To get a leverage on minimal ellipsoids we have to find global structures of the problem that can be efficiently used. Regarding a set $\mathcal{S}$ of Pauli strings as the representation of an algebra is along those lines. To this end, we introduce the frustration graph and consider an example.

It is easy to see from the elementary properties of the four Pauli matrices (from now on including the identity) that each possible pair of Pauli strings either commutes or anticommutes. For a set of strings, this information can be encoded in a graph G, where each vertex represents a string and an edge is drawn whenever two strings anticommute. We refer to this graph as a "frustration graph." Basic examples include the graphs shown in Fig. 1. For example, consider the third graph from the top in Fig. 1. This example was built with Pauli strings

$$S_1 = X \otimes Y, \quad S_2 = Z \otimes Z, \quad \text{and} \quad S_3 = Z \otimes Y. \tag{4}$$

The strings S_1 and S_2 commute, whereas the string S_3 anticommutes with both S_1 and S_2. The joint numerical range is depicted next to it and arises from the intersection of two cylinders. For completeness, it makes sense to regard a cylinder as an asymptotic ellipsoid with one of its principal axes approaching infinity.

Note that fixing a graph G does not uniquely fix the set of strings representing it, and there are more than only unitary degrees of freedom in them. In this sense, there are more sets of strings than there are graphs. For example, any triple of strings will by construction give one of the graphs shown in Fig. 1.

For the questions considered in this work, we can, however, make a basic proposition, formulated in more detail in Theorem 3. It states that the radius of a minimal ellipsoid will be the same across all possible sets of strings representing the same graph.

Proposition 1. Let $\mathcal{S}_1$ and $\mathcal{S}_2$ be sets of Pauli strings with the same frustration graph. Then we have that for any ellipsoid $\mathcal{E}_r(w)$,

$$\mathcal{E}_r(w) \supseteq J(\mathcal{S}_1) \quad \text{if and only if} \quad \mathcal{E}_r(w) \supseteq J(\mathcal{S}_2). \tag{5}$$

In other words, we can turn to investigating structures on a graph G rather than on an explicit set of strings. This can be done by our introducing an algebraic framework. For a given graph G, we will consider operators with the following abstract algebraic properties:

(i) $S_i = S_i^*$.
(ii) $S_i^2 = \mathbb{I}$.
(iii) $S_i^2 \leq \mathbb{I}$.
(iv) $\{S_i, S_j\} = 0$ if $i \sim j$.
(v) $[S_i, S_j] = 0$ if $i \nsim j$.

where $i \sim j$ denotes vertices that are connected by an edge in a given graph G, i.e., i and j are adjacent.

It is clear that Pauli strings will obey all these properties. To investigate bounds on the radius of a minimal ellipsoid, we can, however, turn things around and consider all sets of operators fulfilling these conditions, or at least some of them. By this, we get a constructive tool for setting up relaxations of the joint numerical range. The detailed discussion of such operator representations of a graph is the mathematical core of this work.

Definition 1. For a given graph G, a set $\{S_i\}$ of operators in some Hilbert space $\mathcal{H}$ will be called

(a) a "self-adjoint unitary representation for anticommutativity" (SAURA) if (i), (ii), and (iv) hold. The set of all SAURAs will be denoted by $\mathcal{S}_a(G)$.
(b) a "self-adjoint unitary representation" (SAUR) if (i), (ii), (iv), and (v) hold. The set of all SAURs will be denoted by $\mathcal{S}_{ac}(G)$.
(c) a "self-adjoint representation for anticommutativity" (SARA) if (i), (iii), and (iv) hold. The set of all SARAs will be denoted by $\mathcal{S}_a^{\leq}(G)$.
(d) a "self-adjoint representation" (SAR) if (i), (iii), (iv), and (v) hold. The set of all SARs will be denoted by $\mathcal{S}_{ac}^{\leq}(G)$.

It is clear from the definition above that the different sets of graph representations include each other, i.e., every SAUR is a SAR and a SAURA, and they are all a SARA. This can be captured in the diagram

$$\begin{array}{ccc} \mathcal{S}_a^{\leq}(G) & \supseteq & \mathcal{S}_a(G) \\ \cup\mathrel{|} & & \cup\mathrel{|} \\ \mathcal{S}_{ac}^{\leq}(G) & \supseteq & \mathcal{S}_{ac}(G) \end{array}$$

One can also consider the C^* algebras generated by the different sets of relations. Each of these algebras naturally comes with a state space too, and hence also with a joint numerical range. These joint numerical ranges are by construction outer approximations to the joint numerical range of an explicit set of Pauli strings. The algebra generated by all SAURs is known as quasi Clifford algebra [42]. It is a finite-dimensional algebra and can be seen as a generalization of the Clifford algebra in the sense that we obtain the Clifford algebras as the subcases with a fully connected graph. The representation theory of this object was worked out in Refs. [42,43], and a brief summary can be found in Ref. [31]. In a nutshell, we have that the Pauli strings with which we started are exactly generators of representations of this algebra. Bounds on minimal ellipsoids derived for this algebra are optimal. Bounds arising from consideration of the other algebras give relaxations, i.e., upper bounds on the radius.

The algebra corresponding to all SAURAs can generally be infinite dimensional, yet still separable. As we show later (Lemma 4), the algebra corresponding to a SAR can be understood as the tensor product of the quasi Clifford algebra of the SAURs with a classical (i.e., commuting) algebra. A corresponding result for the algebra corresponding to a SAURA does not hold however.

For a set Ω of operator representations of a graph, where each representation $\mathcal{S}$ acts on a Hilbert space $\mathcal{H}_{\mathcal{S}}$, we can extend the notion of a joint numerical range by considering

$$\mathcal{J}(\Omega) := \left\{ \left(\langle S_i \rangle_\rho\right) \mid \mathcal{S} = \{S_i\} \in \Omega, \rho \in \mathcal{D}(\mathcal{H}_{\mathcal{S}}) \right\}, \quad (6)$$

which is still a subset of $\mathbb{R}^n$, but now containing all possible tuples of expectations attainable by the set of operators corresponding to a particular operator representation. To analyze ellipsoids, it makes sense to also consider the set of squared expectations

$$\mathcal{Q}(\Omega) := \left\{ \left(\langle S_i \rangle_\rho^2\right) \mid \mathcal{S} = \{S_i\} \in \Omega, \rho \in \mathcal{D}(\mathcal{H}_{\mathcal{S}}) \right\}. \quad (7)$$

Given this set, the minimal radius of an ellipsoid [recall Eq. (3)] corresponding to some w is the square root of the maximal value of a linear functional

$$q(\Omega, w) := \sup_{(v_i) \in \mathcal{Q}(\Omega)} \sum_i w_i v_i. \quad (8)$$

In the spheroidal case, when all elements of w are just 1, we omit w in the notation and write $q(\Omega)$. Furthermore, we denote by $\overline{\mathcal{Q}}(\Omega)$ the convex hull of $\mathcal{Q}(\Omega)$. If Ω contains only one element, say, $\Omega = \{x\}$, we abuse notation and write $q(x)$ instead of $q(\{x\})$.

For Ω a $\mathcal{S}_{ac}(G)$, $\mathcal{S}_{ac}^{\leq}(G)$, $\mathcal{S}_a(G)$, or $\mathcal{S}_a^{\leq}(G)$, it holds that

$$\mathcal{J}(\Omega) = \{(\pm\sqrt{q_i}) | (q_i) \in \mathcal{Q}(\Omega)\}, \quad (9)$$

since $\{\pm S_i\} \in \Omega$ if $\{S_i\} \in \Omega$. In this case, the characterization of $\mathcal{J}(\Omega)$ is equivalent to the characterization of $\mathcal{Q}(\Omega)$. $\mathcal{J}(\Omega)$ is always convex and contains what is called the "stable set polytope" STAB(G), which, in those four cases, is given by the convex hull of the set

$$\{(v_i) \mid v_i v_j = 0 \text{ if } i \sim j, v_i, v_j \in \{0,1\}\}.$$

Equation (8) basically states that the full structure of ellipsoids encompassing the different $\mathcal{J}(\Omega)$, and by this also any $\mathcal{J}(\mathcal{S})$ of interest, is encoded in the convex hulls of the different $\mathcal{Q}(\Omega)$.

Now we state our main results and explain the structure of the paper.

Proposition 2. (Main results) Let G be a graph. Let STAB(G) be its stable set polytope and let TH(G) be its Lovász theta body. For $\mathcal{Q}$ evaluated on different representations of G, as introduced above, we have the following ordering relations:

$$\mathrm{STAB}(G) \overset{(a)}{\subseteq} \begin{matrix} \overline{\mathcal{Q}}\left(\mathcal{S}_{ac}(G)\right) \\ \|_{(b)} \\ \overline{\mathcal{Q}}\left(\mathcal{S}_{ac}^{\leq}(G)\right) \end{matrix} \overset{(c)}{\subseteq} \begin{matrix} \mathcal{Q}\left(\mathcal{S}_{a}(G)\right) \\ \|_{(d)} \\ \mathcal{Q}\left(\mathcal{S}_{a}^{\leq}(G)\right) \end{matrix} \overset{(e)}{=} \mathrm{TH}(G), \tag{10}$$

with the Lovász theta body defined as

$$\mathrm{TH}(G) = \{|\langle\phi_0|v_i\rangle|^2 \mid \langle v_i|v_i\rangle = 1, \langle v_i|v_j\rangle = 0 \text{ if } i \sim j\},$$

where $|\phi_0\rangle$ is an arbitrary but fixed normalized vector in $\mathbf{R}^n$.

Consequently, for any non-negative weight vector w,

$$\alpha(G,w) \leq \begin{matrix} q\left(\mathcal{S}_{ac}(G), w\right) \\ \| \\ q\left(\mathcal{S}_{ac}^{\leq}(G), w\right) \end{matrix} \leq \begin{matrix} q\left(\mathcal{S}_{a}(G), w\right) \\ \| \\ q\left(\mathcal{S}_{a}^{\leq}(G), w\right) \end{matrix} = \vartheta(G,w), \tag{11}$$

where $\alpha(G,w) = q(\mathrm{STAB}(G), w)$ and $\vartheta(G,w) = q(\mathrm{TH}(G), w)$ are the weighted independence number and Lovász number of G, and $q\left(\mathcal{S}_{ac}(G), w\right)$ is denoted as $\beta(G,w)$ later.

The equality of $\mathcal{Q}\left(\mathcal{S}_{ac}(G)\right)$ and $\mathcal{Q}\left(\mathcal{S}_{ac}^{\leq}(G)\right)$ [(b) in Eq. (10)] and that of $\mathcal{Q}\left(\mathcal{S}_{a}(G)\right)$ and $\mathcal{Q}\left(\mathcal{S}_{a}^{\leq}(G)\right)$ [(d) in Eq. (10)] are outlined in Sec. VI as Theorems 11 and 10, respectively. Hence, we can focus the main part of our investigations on SAURAs (Sec. III) and SAURs (Sec. IV).

A relation between $q\left(\mathcal{S}_{ac}(G), w\right)$ and $\vartheta(G,w)$ was described in Refs. [31,40]. From the algebraic perspective of this work, this relation is directly captured by the fact that $\overline{\mathcal{Q}}\left(\mathcal{S}_{ac}(G)\right)$ is contained in $\mathrm{TH}(G)$, and their equivalence [(b) in Eq. (10)] is summarized as Theorem 1 in Sec. III. In Sec. V, we prove that the inclusion of $\mathrm{STAB}(G)$ in $\mathcal{Q}\left(\mathcal{S}_{ac}(G)\right)$ can be strict for some graphs, which implies that $\beta(G,w)$ is a new graph parameter. For this, we have to firstly show in Theorem 3 in Sec. IV that $\mathcal{Q}\left(\mathcal{S}_{ac}(G)\right) = \mathcal{Q}\left(\{S_i\}\right)$ for $\{S_i\}$ to be any SAUR of G. We then continue to study the properties of the β number under graph operations in Sec. V; more explicitly, the properties for graph additions as in Theorems 4 and 5, for graph products in Theorems 6 and 7, for edge removal in Theorem 8, and for cycle graphs in Theorem 9. Finally, we apply those results to obtain better bounds than previous ones for uncertainty relations as in Thereom 12, and for ground-state energy as in Theorem 13.

Establishing a bridge to the Lovász theta body $\mathrm{TH}(G)$ and the Lovász number, as described in Proposition 2, is especially interesting from a numerical perspective since $\vartheta(G,w)$ can be computed via semidefinite programming (SDP). Using this as a tool for outer bounds is advantageous since the size of this SDP scales with n, i.e., the number of vertices of G, and by this ultimately with the number of strings in a set $\mathcal{S}$. This has to be contrasted with the problem of computing ground-state energies, i.e., hyperplanes of $J(\mathcal{S})$, whose size scales with the Hilbert space dimension 2^n, where n is the length of the strings.

Furthermore, for a given set of observables $\{S_i\}$, there is a complete hierarchy of SDP relaxations for $q\left(\{S_i\}\right)$ as explained in Appendix B. Two practical see-saw methods for the numerical estimation are also provided in Appendix B. Finally, the estimation can be improved once we know the purity of the state, as discussed in Appendix A.

III. SELF-ADJOINT UNITARY REPRESENTATION FOR ANTICOMMUTATIVITY

As introduced in Sec. II, for a given graph G, a set $\{S_i\}$ of self-adjoint unitaries is said to be a SAURA of G if $i \sim j$ implies that $\{S_i, S_j\} = 0$. An essential task is to characterize $q\left(\mathcal{S}_a(G)\right)$ and $\mathcal{Q}\left(\mathcal{S}_a(G)\right)$.

Lemma 1. (See Ref. [31]) For any graph G, it holds that

$$\alpha(G) \leq q\left(\mathcal{S}_a(G)\right) \leq \vartheta(G). \tag{12}$$

The relation $q\left(\{S_i\}\right) \geq \alpha(G)$ for any SAUR $\{S_i\}$ of a graph G can be directly proven by choosing the state ρ as a common eigenstate of a set of the commuting observables from S_i, where i ranges over a maximal independent set of G. For any graph G, it holds that $\alpha(G) \leq \vartheta(G)$. In the case that G is a perfect graph, we have $\alpha(G) = \vartheta(G)$ [44]. Hence, the upper bound in Eq. (12) is tight for perfect graphs. Especially, in the case that G is a clique graph with n vertices where any two vertices are connected, the relation $q\left(\mathcal{S}_a(G)\right) = 1$ holds. For a given set of observables, numerical estimation of $q\left(\{S_i\}\right)$ can, in principle, provide a more precise bound. Different numerical methods to estimate $q\left(\{S_i\}\right)$ are presented in Appendix B. Here we take the graph-theoretic approach, and provide an exact characterization of $q\left(\mathcal{S}_a(G)\right)$ and $\mathcal{Q}\left(\mathcal{S}_a(G)\right)$.

The graph-theoretic approach has been explored extensively in quantum contextuality [45], where the orthogonality representation (OR) of a graph is used [46]. For a given graph with n vertices, a set of unit vectors $\{|v_i\rangle\}_{i=1}^n$ is said to be an OR of the graph G if $\langle v_i|v_j\rangle = 0$ when $i \sim j$. An OR of a given graph implies a SAURA of the same graph.

Lemma 2. For a given set of d-dimensional vectors $\{\langle v_i| = (v_{i1}, \ldots, v_{id})\}$, if we denote $S_i = \sum_k v_{ik} A_k$, where $\{A_k\}_{k=1}^d$ is a set of anticommuting self-adjoint unitaries, it holds that $\{S_i, S_j^\dagger\}/2 = \langle v_i|v_j\rangle \mathbb{I}$.

There are indeed self-adjoint unitary representations for anticommutativity of a graph that cannot be constructed from an OR—for example, the operators $\{X\mathbb{I}, Y\mathbb{I}, Z\mathbb{I}, ZZ\}$ and their anticommutativity graph. Indeed, those four operators are linearly independent, but there is no operator that anticommutes with all of them at the same time; hence, there is no anticommuting basis for those four operators. In this sense, there are more SAURAs than ORs of a given graph. Nevertheless, such a construction of SAURAs from ORs is the key step in the following proof.

Theorem 1. $\mathcal{Q}(\mathcal{S}_a(G)) = \mathrm{TH}(G)$ for any graph G.

The proof is provided in Appendix C, as are the proofs for the other results given in the main text. Thus, we have a new physical explanation of the graph parameter $\vartheta(G)$.

Example 1. For the pentagon graph, its Lovász number can be achieved with the state $\langle u| = (1,0,0)$ and the following orthogonal representation $\{|v_i\rangle\}_{i=1}^5$, where

$$\langle v_i| = \left(\tau, \tau' \cos(2\pi i/5), \tau' \sin(2\pi i/5)\right), \tag{13}$$

where $\tau = (1/5)^{1/4}$ and $\tau' = \sqrt{1-\tau^2}$.

Hence, by choosing

$$S_i = \sum_k v_{ik}\sigma_k \text{ for all } i = 1,\ldots,5, \tag{14}$$

$$\rho = (\mathbb{I} + \sigma_1)/2, \tag{15}$$

where $\sigma_1 = X$, $\sigma_2 = Y$, and $\sigma_3 = Z$ are Pauli matrices, we have $\sum_i \langle S_i\rangle_\rho^2 = \sqrt{5}$.

There is another concise proof of Theorem 1. $\langle S_i\rangle_\rho = x\langle v_i|u\rangle$ if we take $\rho = (\mathbb{I} + x\sum_k u_k A_k)/d$, where $|x| \le 1$. We note that $\rho \succeq 0$ is a legal state since the maximal eigenvalue of $\sum_k u_k A_k$ is no more than 1. Thus, $\sum_i w_i \langle S_i\rangle_\rho^2 = x^2 \sum_i w_i(\langle v_i|u\rangle)^2 = x^2\vartheta(G,w)$ by definition. By taking $x = \pm 1$, we complete the proof.

Further results along the same line are provided in Appendix A.

IV. SELF-ADJOINT UNITARY REPRESENTATIONS

The set of operators, where any pair either commutes or anticommutes, plays an important role as exemplified by the Pauli strings. The commutation and anticommutation relations of such a set $\{S_i\}$ can be encoded into a so-called frustration graph G [11,12], where $i \sim j$ if $\{S_i, S_j\} = 0$ and $i \not\sim j$ if $[S_i, S_j] = 0$. By the checking of extensive examples, it is conjectured in Ref. [40] that

$$q(\{S_i\}) = \alpha(G). \tag{16}$$

Whether Eq. (16) can be violated is also an open question in Ref. [31]. Conversely, for a given graph G, we can consider its representation by a set $\{S_i\}$ of self-adjoint unitaries, in the sense that $\{S_i, S_j\} = 0$ if $i \sim j$ and $[S_i, S_j] = 0$ if $i \not\sim j$. This representation is called a "self-adjoint unitary representation" [47]. By taking the graph-theoretic approach instead of starting from a special set, we denote $\beta(G,w) = q(\mathcal{S}_{ac}(G), w)$, where $\mathcal{S}_{ac}(G)$ is the set of all SAURs of G. The conjecture in Eq. (16) is equivalent to $\beta(G) = \alpha(G)$. In Ref. [31], no such example is known where $\beta(G) > \alpha(G)$. To continue, we first introduce the standard SAUR of a given graph, which is defined deductively. The standard SAUR can help us to reduce the complexity of considerations, since we need to focus only on the standard SAUR to obtain $\beta(G)$, as we see later.

Definition 2. For a given graph G and one of its edges (i_0, j_0), other vertices except for i_0 and j_0 can be divided into four groups V_0, V_1, V_2, and V_3, such that

(a) $i \not\sim i_0$ and $i \not\sim j_0$ for any $i \in V_0$.
(b) $i \not\sim i_0$ and $i \sim j_0$ for any $i \in V_1$.
(c) $i \sim i_0$ and $i \sim j_0$ for any $i \in V_2$.
(d) $i \sim i_0$ and $i \not\sim j_0$ for any $i \in V_3$.

The subgraph G' of G with vertices in $\cup_{i=0}^4 V_i$ is said to be a Pauli-(i_0, j_0)-induced subgraph of G

(a) if $i \in V_{k_1}$ and $j \in V_{k_2}$, where $k_1 \neq k_2 \in \{1,2,3\}$, we have $i \sim j$ (or $i \not\sim j$) in G' if and only if $i \not\sim j$ (or $i \sim j$) in G;
(b) otherwise $i \sim j$ in G' if and only if $i \sim j$ in G.

Definition 3. For a given graph G and one of its edges (i_0, j_0), if we denote by G' the Pauli-(i_0, j_0)-induced subgraph of G, from a standard SAUR $\{S_i'\}$ of G', we call the following SAUR a standard SAUR of G:

$$\left(\bigcup_{k=0}^{3} \{\sigma_k \otimes S_i'\}_{i\in V_k}\right) \cup \{X_{i_0} \otimes \mathbb{I}, Z_{j_0} \otimes \mathbb{I}\}. \tag{17}$$

If G has no edge, we assign $\mathbb{I}$ or 1 to all its vertices.

If we take the pentagon C_5 in Fig. 2 as the original graph, and $(1,3)$ as the edge, then the Pauli-$(1,3)$-induced subgraph G' is a triangle. Continually, the Pauli-$(4,5)$-induced subgraph G'' of G' is just the vertex 2. Hence, the standard SAURs $\{S_i''\}$, $\{S_i'\}$, and $\{S_i\}$ of G'', G', and G, respectively, are

$$S_2'' = 1, \quad S_2' = Y, \quad S_4' = X, \quad S_5' = Z, \tag{18}$$

$$S_1 = X\mathbb{I}, \quad S_2 = \mathbb{I}Y, \quad S_3 = Z\mathbb{I}, \quad S_4 = ZX, \quad S_5 = XZ, \tag{19}$$

where we have omitted the symbol of the tensor product, and $X\mathbb{I}$ means $X \otimes \mathbb{I}$, etc.

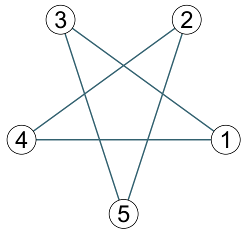

FIG. 2. Pentagon graph C_5.

Theorem 2 (See Ref. [47]). For a given graph G, one SAUR $\{S_i\}$, and one standard SAUR $\{\bar{S}_i\}$ of G, there is a unitary U such that $US_iU^\dagger = \bar{S}_i \otimes D_i$, where $\{D_i\}$ is a set of commuting self-adjoint unitaries.

Though different sequences of edges lead to different standard SAURs, Theorem 2 implies that they are in the same dimension and connected by unitaries. The standard SAUR is succinct; however, it loses the information of the symmetry in the graph. To reflect the structure of the graph, we introduce the edge SAUR.

Definition 4. For a given directed graph $\hat{G}$ with n vertices and the edge set E, the set of self-adjoint operators $\{A_i\}_{i=1}^n$, with $A_i = \otimes_{e\in E} O_{e,i}$, is called the "edge SAUR of $\hat{G}$," where $O_{e,i} = X$ if i is the start of e and $O_{e,i} = Z$ if i is the end of e, otherwise $O_{e,i} = \mathbb{I}$.

For an undirected G, we can lift the concept of an edge SAUR by simply choosing directions. The resulting representation is indeed unique. Switching between different choices of directions results in permutation of X's and Z's. Since every edge corresponds to a single qubit in a edge SAUR, this operation corresponds to a unitary transformation. For different SAURs of the same graph G, their joint expectation values are related.

Theorem 3. For a given graph G, $q(\{S_i\}) = q\left(\{\bar{S}_i\}\right)$, where $\{S_i\}$ is a SAUR of G and $\{\bar{S}_i\}$ is a standard SAUR.

Hence, we have $\beta(G) = q\left(\{\bar{S}_i\}\right)$, where $\{\bar{S}_i\}$ is any standard SAUR of G. A similar result of Theorem 3 for the weighted version can be proven in the same way. Consequently, $\mathcal{Q}(\mathcal{S}_{ac}(G)) = \mathcal{Q}(\{S_i\})$, where $\{S_i\}$ is any SAUR of G. However, $\mathcal{J}(\mathcal{S}_{ac}(G))$ might be strictly larger than $\mathcal{J}(\{S_i\})$ due to the sign of each expectation value. To recover the whole set of $\mathcal{J}(\mathcal{S}_{ac}(G))$, it is enough to consider the complete SAUR as defined below.

Definition 5. For a given graph G with n vertices and its standard SAUR $\{\bar{S}_i\}$, the set $\{S_i\}$ consisting of

$$S_i = \bar{S}_i \otimes \left(\bigotimes_{k=1}^{n} Z^{\delta_{ik}}\right) \tag{20}$$

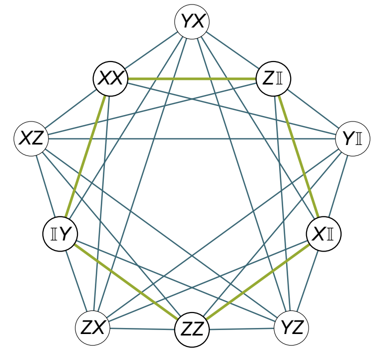

FIG. 3. A graph G_{10} with ten vertices and one of its standard realizations, which contains a pentagon C_5 as an induced subgraph (thick green lines).

is said to be a complete SAUR, where $\delta_{ik} = 1$ if $i = k$, otherwise $\delta_{ik} = 0$.

As we can see, the auxiliary part $\{\otimes_{k=1}^n Z^{\delta_{ik}}\}$ can recover all signs in $\{-1, 1\}^{\otimes n}$. Effectively, this provides a cover of $\mathcal{J}(\mathcal{S}_{ac}(G))$ with multiple copies of $\mathcal{J}\left(\{\bar{S}_i\}\right)$. Generally, $\mathcal{J}\left(\{\bar{S}_i\}\right)$ can be neither point symmetric nor reflection symmetric, but $\mathcal{J}(\mathcal{S}_{ac}(G))$ has both point and reflection symmetries.

V. THE β PARAMETER

For the characterization of the graph parameter $\beta(G)$, we consider some properties of it in this section. First, we show that $\beta(G)$ is indeed different from $\alpha(G)$, although it can occur that $\alpha(G) = \beta(G)$ for certain graphs.

Corollary 1. For the graph G_{10} and C_5 in Fig. 3,

$$\beta(G_{10}) = \alpha(G_{10}) = \beta(C_5) = \alpha(C_5) = 2. \tag{21}$$

However, the conjecture in Eq. (16) is not true generally. A simple counterexample is the antiheptagon and its standard SAUR as shown in Fig. 4. To be more explicit, the seven operators are

$$S_1 = ZZ\mathbb{I},\quad S_2 = Z\mathbb{I}\mathbb{I},\quad S_3 = \mathbb{I}X\mathbb{I},\quad S_4 = X\mathbb{I}\mathbb{I},$$
$$S_5 = XZX,\quad S_6 = YZZ,\quad S_7 = YYY. \tag{22}$$

It can be checked by hand that these operators form one standard SAUR of $\bar{C}_7$, and $\alpha(\bar{C}_7) = 2$.

Let $\rho = |v\rangle\langle v|$ be the state that corresponds to the largest eigenvector of $\sum_i S_i$. With a little bit more handwork, or by using a computer algebra system, one can check that

$$\sum \langle S_i\rangle_\rho^2 = (9 + 4\sqrt{2})/7 \approx 2.09384 > 2 = \alpha(\bar{C}_7), \tag{23}$$

which disproves the conjecture in Eq. (16). Besides, $\vartheta(\bar{C}_7) = 1 + 1/\cos(\pi/7) \approx 2.10992$. Thus, in general,

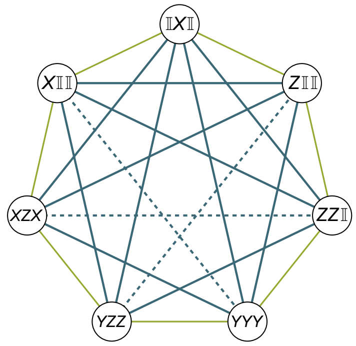

FIG. 4. Graph of the counterexample and its SAUR. A pair of observables anticommute when the corresponding vertices are connected by an edge in the graph of an antiheptagon $\bar{C}_7$ (all blue lines) and commute when they are connected by an edge in the graph of a heptagon C_7 (thin green lines). The subgraph of $\bar{C}_7$ (solid blue lines) is named as "G_7."

$\alpha(G)$, $\beta(G)$, and $\vartheta(G)$ ($\alpha(G) \le \beta(G) \le \vartheta(G)$) are indeed three different graph parameters.

Then we consider properties of the β number under graph operations, e.g., the addition, graph products such as the lexicographic product, and the XOR product. Those properties are helpful for the estimation of the β number for large graphs, which might be impossible with the numerical methods.

A. Additions and products of graphs

Theorem 4. For a given graph G that can be divided into two subgraphs G_1 and G_2 where all vertices in G_1 are connected with all vertices in G_2, then $\beta(G) = \max\{\beta(G_1), \beta(G_2)\}$.

Corollary 2. If we add one new vertex to a graph G and obtain a graph G' in the way that the new vertex is connected to all vertices in G, then $\beta(G') = \beta(G)$.

Theorem 5. For a given graph G that can be divided into two subgraphs G_1 and G_2 where any vertex in G_1 is disconnected from any vertex in G_2, $\beta(G) = \beta(G_1) + \beta(G_2)$.

For two given graphs G_1 and G_2, we denote by $G_1[G_2]$ their lexicographic product, whose vertex set is the Cartesian product of the graphs' vertex sets and then $(i_1,j_1) \sim (i_2,j_2)$ if $i_1 \sim i_2$, or $j_1 \sim j_2$ when $i_1 = i_2$.

Theorem 6. For two given graphs G_1 and G_2, $\beta(G)$ is multiplicative under the lexicographic product: $\beta(G_1[G_2]) = \beta(G_1)\beta(G_2)$.

For any large graph with decomposition into small graphs with known β numbers through the two addition operations and lexicographic product, its exact β number can be obtained. For example, if we take the lexicographic product of five $\bar{C}_7$'s, i.e., $G = \bar{C}_7^{[\,]5}$, then $\beta(G) = \beta(\bar{C}_7)^5 \approx 40.2452$. However, $\alpha(G) = \alpha(\bar{C}_7)^5 = 32$ and $\vartheta(G) = \vartheta(\bar{C}_7)^5 \approx 41.8144$ since the latter two parameters are multiplicative under the lexicographic product, too [48–50]. Hence, the integer parts of $\beta(G)$, $\alpha(G)$, and $\vartheta(G)$ can be all different. This answers an open question in Ref. [31] in the negative: there are indeed graphs with β number strictly larger than the independence number, and the gap between them can be arbitrarily large.

The tensor product of systems is often relevant in quantum mechanics. We denote by G the anticommutativity and commutativity graph corresponding to the tensor product of the SAURs of G_1 and G_2. We can directly verify that G is the XOR product of G_1 and G_2, i.e., $(i_1,j_1) \sim (i_2,j_2)$ if and only if only one of $i_1 \sim i_2$ and $j_1 \sim j_2$ holds. In this case, we denote $G = G_1 \times G_2$.

Theorem 7. For any pair of graphs G_1 and G_2, $\beta(G_1 \times G_2) \ge \beta(G_1)\beta(G_2)$.

B. Removal of edges

The removal of one edge is also one basic graph operation, which can relate different graph products. One important property shared by the independence number and the Lovász number is that they do not decrease under edge removal. However, this does not hold for the β number. Here we take $\bar{C}_7$ and its subgraph G_7 (see Fig. 4) as an example, where the aforementioned properties of the β number play a role.

Theorem 8. $\beta(G_7) = 2 < \beta(\bar{C}_7)$.

Proof. Note that G_7 is isomorphic to an induced subgraph of $C_5[K_2]$, where K_2 is just one edge. Thus,

$$\beta(G_7) \le \beta(C_5)\beta(K_2) = 2. \tag{24}$$

On the other hand, $\beta(G_7) \ge \alpha(G_7) = 2$, which completes the proof. ∎

Although the β number is between the independence number and the Lovász number, its behavior under edge removal is rather strange. Nevertheless, the β number does not increase under vertex removal, the same property as for the independence number and the Lovász number. More explicitly, $\beta(G') \le \beta(G)$ if G' is an induced subgraph of G.

C. Cycles and anticycles

For a perfect graph G, we know that $\alpha(G) = \vartheta(G) = \alpha^\star(G)$, which implies that $\alpha(G) = \beta(G) = \vartheta(G) = \alpha^\star(G)$. For imperfect graphs, odd cycles and odd anticycles are

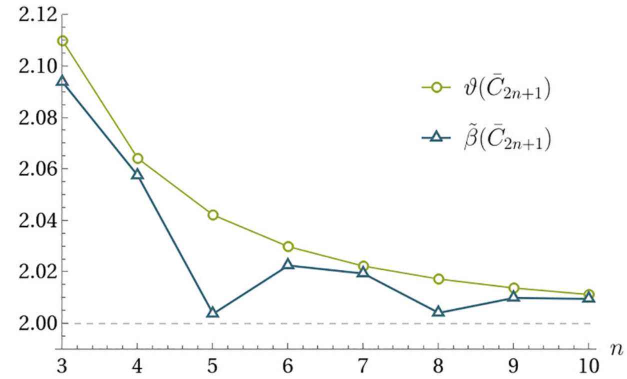

FIG. 5. The estimation $\tilde{\beta}(\bar{C}_{2n+1})$ of $\beta(\bar{C}_{2n+1})$ in comparison with $\vartheta(\bar{C}_{2n+1})$. For each estimation, we used the second see-saw method with 500 rounds of iteration.

basic building blocks. It turns out that the following theorem holds.

Theorem 9. $\beta(C_m) = \alpha(C_m)$, which consequently implies that $\overline{\mathcal{Q}}(\mathcal{S}_{ac}(C_m)) = \mathrm{STAB}(C_m)$.

Numerically, we have $\vartheta(\bar{C}_{2n+1}) > \beta(\bar{C}_{2n+1}) > \alpha(\bar{C}_{2n+1}) = 2$ for $n \leq 10$ (see Fig. 5 for more details); for any graph G with no more than nine vertices, if $\beta(G) > \alpha(G)$, then G has either $\bar{C}_7$ or $\bar{C}_9$ as an induced subgraph.

Although these observations might suggest the conjecture that $\overline{\mathcal{Q}}(\mathcal{S}_{ac}(G)) \supsetneq \mathrm{STAB}(G)$ *if and only if* G *has some* $\bar{C}_{2n+1}$ *as an induced subgraph, where* $n \geq 3$, it is refuted by a very recent counterexample [51].

VI. SELF-ADJOINT REPRESENTATIONS AND RETURN TO JOINT NUMERICAL RANGE BEYOND NONUNITARY OBSERVABLES

Whether in a SAURA or in a SAUR, we have considered only self-adjoint unitaries, which can limit the range of applications. We generalize our setting to nonunitary operators in this section.

Definition 6. For a given graph G, a set of operators $\{A_i\}$ is said to be a SARA of G if each A_i is self-adjoint, $A_i^2 \leq \mathbb{I}$, $\{A_i, A_j\} = 0$ when $i \sim j$. Furthermore, if $[A_i, A_j] = 0$ whenever $i \not\sim j$, $\{A_i\}$ is said to be a SAR of G.

For a given graph G, denote by $\mathcal{S}_a^{\leq}(G)$ the set of all its SARAs and denote by $\mathcal{S}_{ac}^{\leq}(G)$ the set of all its SARs. By definition, $\mathcal{S}_a(G) \subseteq \mathcal{S}_a^{\leq}(G)$ and $\mathcal{S}_{ac}(G) \subseteq \mathcal{S}_{ac}^{\leq}(G)$. Surprisingly, maximizing the function q in Eq. (8) over $\mathcal{S}_a^{\leq}(G)$ instead of $\mathcal{S}_a(G)$ does not result in a larger value, and the same is true for $\mathcal{S}_{ac}^{\leq}(G)$ and $\mathcal{S}_{ac}(G)$. This is expressed more explicitly in the following theorems.

Theorem 10. $\mathcal{Q}\left(\mathcal{S}_a^{\leq}(G)\right) = \mathcal{Q}\left(\mathcal{S}_a G\right) = \mathrm{TH}(G)$.

Theorem 11. $\mathcal{Q}\left(\mathcal{S}_{ac}^{\leq}(G)\right) = \mathcal{Q}\left(\mathcal{S}_{ac} G\right)$.

A set is said to be star-convex if all the points, that are on the line segment between the origin and any point in the set are in the set too. It turns out that $\mathcal{Q}\left(\mathcal{S}_{ac}(G)\right)$ is indeed star-convex. More details are provided in Appendix C.

VII. APPLICATIONS

As an application, we provide bounds for sum uncertainty relations among sets of observables with certain anticommutation or commutation relations.

Theorem 12. For a given set of observables $\{A_i\}_{i=1}^n$ that is a SARA of G, we have

$$\sum_i \Delta^2(A_i) \geq \lambda_{\min} - \vartheta(G, \lambda), \tag{25}$$

where $\lambda_{\min}$ is the minimal singular value of $\sum_i A_i^2$, and $\lambda = (a_1^2, \ldots, a_n^2)$, with a_i the maximal eigenvalue of A_i. Besides, if $\{A_i\}$ is a SAR of G, then

$$\sum_i \Delta^2(A_i) \geq \lambda_{\min} - \beta(G, \lambda). \tag{26}$$

For a given set of observables $\{A_i\}_{i=1}^n$, the estimation of $\lambda_{\min}$ is a relatively easy problem. If each A_i has only two outcomes $\pm a_i$, then $\lambda_{\min} = \sum_i a_i^2$. In comparison with the similar application on uncertainty relations in Ref. [40], our results are not limited to dichotomic observables. Besides, the inequality (26) is tighter in general.

Our results can also be used to estimate the ground-state energy, which is of great interest in quantum many-body systems [10,29]. For a given frustration graph G with n vertices, the dimension of the system to realize it is exponential in n [42]. This can make the problem notoriously challenging to solve.

Theorem 13. For a given set of Pauli strings $\{A_i\}_{i=1}^n$ whose frustration graph is G,

$$\left(\sum_i a_i \langle A_i \rangle_\rho\right)^2 \leq \min_w \left(\sum_i a_i^2/w_i\right)\beta(G, w) \tag{27}$$

$$\leq \min_w \left(\sum_i a_i^2/w_i\right)\vartheta(G, w) \tag{28}$$

for any state ρ and any real coefficients a_i.

Proof. By using the Cauchy-Schwarz inequality, we have

$$\Big(\sum_i a_i \langle A_i\rangle\Big)^2 \le \Big(\sum_i a_i^2/w_i\Big)\Big(\sum_i w_i \langle A_i\rangle^2\Big) \tag{29}$$

$$\le \Big(\sum_i a_i^2/w_i\Big)\beta(G,w), \tag{30}$$

where w_i's are positive. Thus, the inequality still holds when we take the minimization over possible w. ■

Especially, we can set $w_i = |a_i|^t$ for $t = 0, 1, 2$. For $t = 0$, we recover the result in Ref. [31] with Eq. (28) for Pauli strings, which is less tight than the one in Eq. (27) in general. However, when some a_i's are much larger than others, much better performance can be obtained by taking $t = 1$ or $t = 2$. For example, $a_1 = 1$ and all the a_i's are 0, and then the results for $t = 0$ and $t = 1$ are $\vartheta(G)$ and 1, respectively. And $\vartheta(G)$ can be much larger than 1 for a big graph G. In general, a tighter bound can be obtained from Eq. (29) than the case where $w_i = |a_i|^t$ for $t = 0, 1, 2$. More precisely, the bound reads

$$\min_w \max_{v\in Q} \Big(\sum_i a_i^2/w_i\Big)\Big(\sum_i w_i v_i\Big), \tag{31}$$

where $Q = \mathrm{TH}(G)$ or $Q = \overline{\mathcal{Q}}(\mathcal{S}_{ac}(G))$. If G is either a perfect graph or a cycle, $Q = \overline{\mathcal{Q}}(\mathcal{S}_{ac}(G)) = \mathrm{STAB}(G)$. This becomes a min-max problem of size n, which is relatively much easier than the original problem.

We take the Hamiltonian $H = \sum_{i=1}^7 A_i$ on 14 qubits as the first example, where

$$\begin{aligned} &A_1 = Z_1Z_2Z_3Z_4, \quad A_2 = Z_5Z_6Z_7Z_8,\\ &A_3 = X_1Z_9Z_{10}Z_{11}, \quad A_4 = X_2X_5Z_{12}Z_{13},\\ &A_5 = X_3X_6X_9Z_{14}, \quad A_6 = X_4X_7X_{10}X_{12},\\ &A_7 = X_8X_{11}X_{13}X_{14}. \end{aligned} \tag{32}$$

This set $\{A_i\}_{i=1}^7$ is the edge SAUR of $\bar{C}_7$ as in Fig. 4. Direct calculation shows that the minimal and maximal eigenvalues of H are -3.828427 and 3.828427, respectively. This agrees with the upper bound in Eq. (30) by setting the w_i's equal to 1, i.e., $\sqrt{7\beta(\bar{C}_7)} = 1 + 2\sqrt{2}$.

We take the Hamiltonian $H = \sum_{i=1}^9 A_i$ on 27 qubits as the second example, where

$$\begin{aligned} &A_1 = Z_1Z_2Z_3Z_4Z_5Z_6, \quad A_2 = Z_7Z_8Z_9Z_{10}Z_{11}Z_{12},\\ &A_3 = X_1Z_{13}Z_{14}Z_{15}Z_{16}Z_{17}, \quad A_4 = X_2X_7Z_{18}Z_{19}Z_{20}Z_{21},\\ &A_5 = X_3X_8X_{13}Z_{22}Z_{23}Z_{24}, \quad A_6 = X_4X_9X_{14}X_{18}Z_{25}Z_{26},\\ &A_7 = X_5X_{10}X_{15}X_{19}X_{22}Z_{27}, \quad A_8 = X_6X_{11}X_{16}X_{20}X_{23}X_{25},\\ &A_9 = X_{12}X_{17}X_{21}X_{24}X_{26}X_{27}. \end{aligned} \tag{33}$$

This set $\{A_i\}_{i=1}^9$ is the edge SAUR of $\bar{C}_9$. Direct calculation of the minimal and maximal eigenvalues of H is hard since its dimension is 2^{27}. An easy numerical calculation shows that $\beta(\bar{C}_9) = 2.057505$, which implies that the maximal singular value of H is bounded by $\sqrt{9\beta(\bar{C}_9)} = 4.303201$, where we have used Eq. (30) by setting the w_i's equal to 1. This bound is tight, as we can verify by converting $\{A_i\}$ into the standard SAUR with an auxiliary system as in Theorem 2.

For a general frustration graph with n vertices, the dimension of the edge SAUR is $2^{|E|}$, where $|E|$ is the number of edges in the frustration graph, and typically $|E| = O(n^2)$. Hence, the direct evaluation of the ground-state energy is in dimension $2^{O(n^2)}$. The estimation as in Eq. (30) deals only with a graph with n vertices, which could be much simpler.

VIII. CONCLUSION AND DISCUSSION

The deep connection between sums of squares of expectations of Pauli strings, on the one hand, and parameters of the corresponding frustration graph, on the other, was observed and successfully used in Refs. [31,40]. In Ref. [40] it was used to derive upper and lower bounds on uncertainty relations in terms of the independence number and in terms of the Lovász number, respectively. Conceptually similar results were used by Hastings and O'Donnell [31] in the context of many-body Hamiltonians. Those initial findings opened up a broader perspective with many new questions to answer, setting one of the starting points for the present work.

We investigate the joint numerical range of a set of Pauli strings, as the general object that encodes the answers to a whole cornucopia of interesting questions, and of which we have here only scratched the surface. In our setting, the previously discussed bounds on sums of squares can be cast in the nice geometrical picture of ellipsoids encompassing $J(S)$. A central finding here, and another starting point for our study, is the insight that the structure of these ellipsoids is determined solely by the frustration graph and not by a particular realization of Pauli strings itself. Because of this, we introduce and investigate the invariant $\beta(G)$ as a new graph parameter. This shift of attention towards the graph then brought us directly to using an algebraic description that takes a particular graph as the input and provides an axiomatically defined algebra as the output. These algebras are known as quasi Clifford algebras, and their investigation goes back to the work of Gastineau-Hills [42,43] in the 1980s, which gave a solid foundation of results on which we could build. Furthermore, dropping parts of these axioms then naturally leads to relaxations and hence ultimately to outer bounds on the joint numerical range. This approach gives rise to what we call here a SARA, a SAURA, and a SAR. In conclusion, we find that taking a graph-theoretic approach instead of focusing on a set of exact operators opened up an unexpectedly rich new perspective leading in many directions.

First, the comparison with the graph-theoretic approach in other fields builds up a channel through which we can convert known results into the research field of joint numerical range. In the current work, the graph-theoretic approach in contextuality leads to the proof of the tight bound for the SAURA case, and the generalization of the SAURA case. Second, the graph-theoretic approach can pick up the most relevant representations and discover new crucial gradients such as purity. In the SAUR case, only after it has been proven that the upper bound is always achievable by the standard representation does it become possible to enumerate graphs to compare the upper bound with other graph parameters. It turned out that the upper-bound β number in the SAUR case is indeed a new graph parameter, which is different from both the independence number and the Lovász number. According to the known evidence, the β number can be used as a quite good approximation of the independence number. Third, the graph-theoretic approach provides another level, i.e., the graph level, to study the joint numerical range. By considering graph operations and special graphs, we can characterize the β number and get the β number for large graphs, or large sets of operators, which might be impossible for direct numerical calculations. Hence, the graph-theoretic approach not only deepens and expands the joint numerical range field but it also connects to other fields such as quantum contextuality and graph theory. In our current work, we have also developed numerical methods for the estimation of the upper bound from below and from above. Finally, we generalized this approach to general self-adjoint operators that do not need to be unitaries.

However, there are still many open problems remaining, some of which we highlight here:

(a) How can we calculate the β number, especially approximate it from above, more efficiently?

(b) The β number is closely related to the algebra generated by the standard SAUR. How can we characterize the β number from the algebraic graph theory? If the graph has the whole algebra as its SAUR, Ref. [52] already has a complete characterization.

(c) With $\otimes$ denoting the OR product of graphs, does $\beta(G_1 \otimes G_2) = \beta(G_1)\beta(G_2)$ hold? If it does, then the β number could be closely related to the Shannon capacity of the graph [53].

(d) Could the graph-theoretic approach be applied to the variance-based criteria for quantum correlations, such as the criterion for entanglement [54]?

(e) How could we develop the graph-theoretic approach for other kinds of uncertainty relation? The fractional packing number $\alpha^\star(G)$ might play an important role, which is defined as the maximum of $\sum_{i=1}^n x_i$, where $x_i \geq 0$ and $\sum_{i\in C} x_i \leq 1$ for any clique C in graph G. For example, for the quantum entropic uncertainty relation of a set of anticommuting self-adjoint unitaries, it is known [55] that $\sum_{i\in C}[1 - H(S_i|\rho)] \leq 1$ holds and $0 \leq H(S_i|\rho) \leq 1$, where $H(S|\rho)$ is the Shannon entropy of the statistics from the two-outcome measurement S with the state ρ. This leads to $\sum_{i=1}^n H(S_i|\rho) \geq n - \alpha^\star(G)$, where G is the anticommutativity graph of $\{S_i\}$.

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APPENDIX A: FURTHER RESULTS CONCERNING SAURA

1. Tighter bound based on purity

Note that the purity can be written as $\operatorname{Tr}\rho^2 = (1 + x^2)/d$, which provides the intuition that the purity of the state could affect the joint expectation values. A direct observation is that $\sum_i \langle S_i\rangle^2 = 0$ always holds for the maximally mixed state. By making use of the information of purity, we can improve the estimation of joint expectation values.

Theorem 14. For a given set of d-dimensional observables $\{S_i\} \in \mathcal{S}_a(G)$, and a state ρ, we have

$$\sum_i \langle S_i \rangle_\rho^2 \leq \min\{[d(\operatorname{Tr}\rho^2) - 1]\vartheta(G), \vartheta(G)\}. \tag{A1}$$

Furthermore, for any given graph G and the purity of the state, the upper bound in Eq. (A1) is always tight.

The discussion at the beginning of this section works as a constructive proof. We remark that $[d(\operatorname{Tr}\rho^2) - 1]\vartheta(G) \leq \vartheta(G)$ always hold when the dimension is 2, as in the case in Example 1. Note that $\operatorname{Tr}\rho^2$ is related to the linear entropy of the state, and the inequality shows how the entropy of the state affects the joint expectation values. It is interesting to see that the linear entropy of the state affects the joint expectation values only when the linear entropy is large enough, i.e., when $\operatorname{Tr}\rho^2 \leq 2/d$. This happens when the temperature of the thermal state is high or when the system is highly entangled with the environment.

2. Relaxation of anticommutation relation

The anticommutation relation of operators leads to their orthogonality in the sense of the trace product. That is, if $\{S_i, S_j\} = 0$, then $\operatorname{Tr} S_iS_j = 0$. However, the converse is not necessarily true, e.g., $S_1 = XX$ and $S_2 = ZZ$. For convenience, denote by $|S\rangle$ the vector obtained by flattening the operator S row by row. With this notation, $\operatorname{Tr} S_iS_j = \langle S_i|S_j\rangle$. As we see later, $\{S_i, S_j\} = 0$ also implies that $\operatorname{Tr} S_i = \operatorname{Tr} S_j = 0$. Hence, $\langle S_i\rangle_\rho = \langle S_i|\tilde{\rho}\rangle$, where $\tilde{\rho} = \rho - \mathbb{I}/d$ and d is the dimension. Note that $\langle\tilde{\rho}|\tilde{\rho}\rangle = \operatorname{Tr}\rho^2 - 1/d$, $\langle S_i|S_i\rangle = d$. By comparison with the definition of the Lovász number, we have a generalization of Theorem 1.

Theorem 15. For a given graph G and its d-dimensional orthogonality representation with $\{S_i\}$ such that $\langle S_i|S_i\rangle = d$ and $\langle S_i|S_j\rangle = 0$, if $i \sim j$, then

$$\sum_i \langle S_i \rangle_\rho^2 \leq [d(\operatorname{Tr}\rho^2) - 1]\vartheta(G). \tag{A2}$$

We have two remarks: First, the constructive proof of Theorem 1 implies that the bound in Theorem 15 is tight whenever $\operatorname{Tr}\rho^2 \leq 2/d$. Second, the results in Lemma 2, Theorems 1 and 15, and the technique of vectorization of matrices give hints to the similarity of the role of $\vartheta(G)$ in quantum contextuality and joint expectation values.

APPENDIX B: NUMERICAL METHODS

The independence number $\alpha(G)$ is an important graph parameter, and has application in the characterization of channel capacity. The calculation of $\alpha(G)$ is nondeterministic polynomial time hard [56], and the calculation of $\vartheta(G)$ is just a semidefinite programming. Thus, $\vartheta(G)$ can be used as an approximation of $\alpha(G)$. Since $\beta(G)$ is a tighter upper bound of $\alpha(G)$ than $\vartheta(G)$, efficient methods to estimate $\beta(G)$ are necessary. As we have proven, $\beta(G) = q\left(\{\bar{S}_i\}\right)$, where $\{\bar{S}_i\}$ is any standard SAUR of G, a more general problem is to estimate $q(\{S_i\})$ for a given set of $\{S_i\}$. For example, there might be only some anticommutation relations in $\{S_i\}$. In this appendix, we provide two efficient see-saw methods to give lower bounds of $\beta(G)$, and one complete hierarchy of semidefinite programming to approximate $\beta(G)$ from the upper bound.

1. Lower bounds

We note that

$$q(\{S_i\}) = \max_\rho \sum_{i=1}^n \operatorname{Tr}[(\rho\otimes\rho)(S_i\otimes S_i)] \tag{B1}$$

$$= \max_\rho \operatorname{Tr}\left[(\rho\otimes\rho)\sum_{i=1}^n (S_i\otimes S_i)\right]. \tag{B2}$$

On the one hand, we have

$$\operatorname{Tr}\left[(\rho_1\otimes\rho_2)\sum_{i=1}^n (S_i\otimes S_i)\right] \leq \left(\sum_{i=1}^n \langle S_i\rangle_{\rho_1}^2 \sum_{i=1}^n \langle S_i\rangle_{\rho_2}^2\right)^{1/2} \leq q(\{S_i\}). \tag{B3}$$

On the other hand,

$$q(\{S_i\}) \leq \max_{\rho_1,\rho_2} \operatorname{Tr}\left[(\rho_1\otimes\rho_2)\sum_{i=1}^n (S_i\otimes S_i)\right]. \tag{B4}$$

Consequently, we have

$$q(\{S_i\}) = \max_{\rho_1,\rho_2} \operatorname{Tr}\left[(\rho_1\otimes\rho_2)\sum_{i=1}^n (S_i\otimes S_i)\right]. \tag{B5}$$

For a given ρ_1, the optimal ρ_2 corresponds to the eigenstate with the maximal singular value of $\sum_{i=1}^n (\operatorname{Tr}\rho_1 S_i)S_i$. Similarly, for a given ρ_2, the optimal ρ_1 corresponds to the eigenstate with the maximal singular value of $\sum_{i=1}^n (\operatorname{Tr}\rho_2 S_i)S_i$. Hence, we can use a see-saw method to estimate $q(\{S_i\})$, where each step is only a singular value decomposition. This see-saw method can be generalized for any polynomial of mean value by consideration of $\rho_1, \ldots, \rho_k$, where k is the order of the polynomial.

Another observation is that

$$q(\{S_i\}) = \max_{\rho,\, c \text{ subject to } ||c||_2=1} \left(\sum_i c_i \langle S_i\rangle_\rho\right)^2, \tag{B6}$$

which leads to another see-saw method for the lower bound. It turns out that for a given ρ, the optimal vector

c is the normalized vector of $(\langle S_i\rangle_\rho)_{i=1}^n$. For a given vector c, the optimal ρ corresponds to the eigenstate with the maximal singular value of $\sum_{i=1}^n c_i S_i$.

Since it is unnecessary to require that $S_i^2 = \mathbb{I}$ in those two methods, they can be naturally extended to the weighted version, i.e., $q(\{S_i\}, w)$.

2. Upper bounds

According to Eq. (B5) and the linearity on $\rho_1 \otimes \rho_2$ as a whole state, we have

$$q(\{S_i\}) = \max_{\gamma\in\mathcal{S}_{\rm sep}} \operatorname{Tr}\left[\gamma \sum_{i=1}^n (S_i \otimes S_i)\right], \tag{B7}$$

where $\mathcal{S}_{\rm sep}$ is the set of separable states.

Our first observation is that the maximum can always be achieved in the case that γ is a pure state, and the set of pure separable states can be fully characterized by the positive partial transpose condition and the rank-1 constraint.

Thus, we can reformulate the optimization into a rank-constrained problem:

$$q(\{S_i\}) = \max_{\gamma} \operatorname{Tr}\left[\gamma \sum_i (S_i \otimes S_i)\right]$$

$$\text{such that } \operatorname{Tr}\gamma = 1, \gamma \succeq 0, \gamma^{T_2} \succeq 0, \tag{B8}$$

$$F_{12}\gamma = \gamma, \tag{B9}$$

$$\operatorname{rank}\gamma = 1, \tag{B10}$$

where F_{12} is the swap operator $\sum_{ij} |ij\rangle\langle ji|$ and T_2 means the partial transpose on the second party.

According to Eq. (B1), the condition in Eq. (B9) can be added without the outcome being changed.

As proposed in Ref. [57], there is a complete hierarchy of relaxation with semidefinite programming for the rank-constrained problem, which leads to such a complete hierarchy for the problem we are considering. However, this technique is not so practical here. If d denotes the dimension of S_i, then the dimension of γ is d^2. The size of the matrix on the kth level is then d^{2k}. Even if $d = 8$ as in the standard SAUR of $\bar{C}_7$, by taking $k = 2$, we have $d^{2k} = 4096$, in which size a semidefinite programming is quite hard for a desktop computer. For practical purposes, we propose the following relaxation of the rank-1 constraints:

$$q(\{S_i\}) = \max_{\gamma} \operatorname{Tr}\left[\gamma \sum_i (S_i \otimes S_i)\right]$$

$$\text{such that } \operatorname{Tr}\gamma = 1, \gamma \succeq 0, \gamma^{T_2} \succeq 0, \tag{B11}$$

$$F_{12}\tau = F_{23}\tau = \tau,$$

$$\operatorname{Tr}_3 \tau = \gamma,$$

which can be seen as the 3/2 level of the hierarchy. This technique is special for our case since the state γ is already two copies of the state in the system of $\{S_i\}$.

Another approach to achieve relaxation of SEP is to add more semidefinite conditions such as the positive partial transpose condition and linear conditions such as an entanglement witness. We refer the reader to Appendix B in Ref. [58] for detailed discussions. The conditions in Eq. (C24) are such an example.

APPENDIX C: PROOFS OF MAIN RESULTS

Theorem 16. $\mathcal{Q}(\mathcal{S}_a(G)) = \mathrm{TH}(G)$ for any graph G.

Proof. To prove this theorem is equivalent to show that $q(\mathcal{S}_a(G), w) = \vartheta(G, w)$ for any non-negative weight vector w. Equation (12) includes already the result that $q(\mathcal{S}_a(G), w) \le \vartheta(G, w)$ when all the elements of w are just 1. For the general non-negative weight vector w, we prove $q\mathcal{S}_a(G), w \le \vartheta(G, w)$ in the proof of Theorem 41.

To show that $q(\mathcal{S}_a(G), w) \ge \vartheta(G, w)$, we construct an exact $\{S_i\} \in \mathcal{S}_a(G)$ such that $q(\{S_i\}, w) = \vartheta(G, w)$.

Denote $\{|v_i\rangle\}_{i=1}^n$ and by $|u\rangle$ the OR of the graph G and the state such that $\vartheta(G, w) = \sum_{i=1}^n w_i |\langle v_i|u\rangle|^2$, which can be assumed to be real without loss of generality. Denote by $\{A_i\}_{i=1}^r$ a set of d-dimensional normalized traceless observables satisfying $\{A_i, A_j\}/2 = \delta_{ij}\mathbb{I}$, where r is the dimension of $\{|v_i\rangle\}_{i=1}^n$. By setting $S_i = \sum_{k=1}^r v_{i,k} A_k$, the S_i's are Hermitian and $\{S_i, S_j\}/2 = \langle v_i|v_j\rangle\mathbb{I}$, which implies that $\{S_i\}$ is a SAURA of G.

For a given state ρ, denote by $\mathcal{M}_\rho$ the matrix whose (i,j)th element is $\sqrt{w_i w_j}\left\langle \{S_i, S_j\}/2\right\rangle_\rho$. In this special case, $\left\langle \{S_i, S_j\}/2\right\rangle_\rho = \langle v_i|v_j\rangle$ which is independent of the exact state ρ. Then $\lambda_{\max}(\mathcal{M}_\rho) = \vartheta(G, w)$. If we denote by $|a\rangle$ the eigenvector of $\mathcal{M}_\rho$ corresponding to the maximal eigenvalue, we have $\langle a|\mathcal{M}_\rho|a\rangle = \vartheta(G, w)$.

Denote by $|s\rangle$ the eigenstate of $\sum_i a_i\sqrt{w_i} S_i$ corresponding to the maximal eigenvalue and $\sigma = |s\rangle\langle s|$. Then

$$\begin{aligned}\sum_i w_i \langle S_i\rangle_\sigma^2 &\ge \left(\sum_i a_i \sqrt{w_i}\,\langle S_i\rangle_\sigma\right)^2 \\ &= \left(\left\langle \sum_i a_i\sqrt{w_i} S_i\right\rangle_\sigma\right)^2 \\ &= \left\langle \left(\sum_i a_i\sqrt{w_i} S_i\right)^2\right\rangle_\sigma \\ &= \vartheta(G, w),\end{aligned} \tag{C1}$$

where the first line is from the Cauchy-Schwarz inequality since $|a\rangle$ is normalized, the third line is from the definition of σ and the last line is from the definition of $|a\rangle$ and the fact that $\mathcal{M}_\rho$ is independent of the state ρ. Finally, we have $q(\mathcal{S}_a(G), w) \ge \vartheta(G, w)$ and we complete the proof. ∎

The construction in Lemma 2 is crucial for the proof, as the last line in Eq. (C1) may not hold for a general SAURA.

Theorem 17. For a given graph G, $q(\{S_i\}) = q\left(\{\bar{S}_i\}\right)$, where $\{S_i\}$ is a SAUR of G and $\{\bar{S}_i\}$ is a standard SAUR.

Proof. From the convexity of $\sum_i \langle S_i\rangle^2$, we know that we need to prove the theorem only for the case that ρ is a pure state $|\psi\rangle\langle\psi|$. Since the D_i's commute with each other, we can assume the D_i's are diagonal matrices. If we denote by d_2 the dimension of the D_i's, then we have the decomposition

$$U|\psi\rangle = \sum_{i=1}^{d_2} \sqrt{p_i}|\phi_i\rangle \otimes |i\rangle, \tag{C2}$$

where $p_i \geq 0$ and $\sum_i p_i = 1$.

Hence,

$$\begin{aligned}\langle S_i\rangle &= \sum_{kl} \sqrt{p_i p_j}\,\langle\phi_k|\bar{S}_i|\phi_l\rangle\langle k|D_i|l\rangle \\ &= \sum_k p_k\langle\phi_k|s_{ik}\bar{S}_i|\phi_k\rangle,\end{aligned} \tag{C3}$$

where $s_{ik} \in \{-1, 1\}$ is the kth diagonal element in D_i.

Then we have

$$\langle S_i\rangle^2 = \left(\sum_k p_k\langle\phi_k|s_{ik}\bar{S}_i|\phi_k\rangle\right)^2 \leq \sum_k p_k\langle\phi_k|\bar{S}_i|\phi_k\rangle^2, \tag{C4}$$

which implies that

$$\begin{aligned}\sum_i \langle S_i\rangle^2 &\leq \sum_k p_k\left(\sum_i |\langle\phi_k|\bar{S}_i|\phi_k\rangle|^2\right) \\ &\leq \max_k \sum_i \langle\phi_k|\bar{S}_i|\phi_k\rangle^2.\end{aligned} \tag{C5}$$

Thus, $q(\{S_i\}) \leq q\left(\{\bar{S}_i\}\right)$.

On the other hand, if we denote by $|\phi\rangle$ the optimal state for $q\left(\{\bar{S}_i\}\right)$ and by $|\psi_0\rangle$ the common eigenstate for the D_i's, then

$$\sum_i \langle S_i\rangle_\rho^2 = \sum_i \langle\phi|\bar{S}_i|\phi\rangle^2, \tag{C6}$$

where $\rho = |\psi\rangle\langle\psi|$ and $|\psi\rangle = U^\dagger[|\phi\rangle \otimes |\psi_0\rangle]$. Thus, we have $q(\{S_i\}) \geq q\left(\{\bar{S}_i\}\right)$. This finishes the proof. ■

Corollary 3. For the graph G_{10} and C_5 in Fig. 3,

$$\beta(G_{10}) = \alpha(G_{10}) = \beta(C_5) = \alpha(C_5) = 2. \tag{C7}$$

Proof. Note that $\beta(G) \geq \alpha(G)$, $\beta(G_{10}) \geq \beta(C_5)$, and $\alpha(G_{10}) = \alpha(C_5) = 2$. We need to prove only that $\beta(G_{10}) = 2$. According to Theorem 3, it is sufficient to consider the standard SAUR of G_{10} as the one in Fig. 3, and we denote it by $\{S_i\}_{i=1}^{10}$.

Because of the convexity of $\sum_i \langle S_i\rangle_\rho^2$ in terms of state ρ, we only need to consider the state to be a pure four-dimensional state:

$$\begin{aligned}|\psi\rangle = \{&\cos\theta_1, e^{it_1}\sin\theta_1\cos\theta_2, e^{it_2}\sin\theta_1\sin\theta_2\cos\theta_3, \\ &e^{it_3}\sin\theta_1\sin\theta_2\sin\theta_3\}.\end{aligned} \tag{C8}$$

A direct calculation shows that

$$\sum_{i=1}^{10} \langle S_i\rangle^2 = 2. \tag{C9}$$

■

The fact that $\beta(C_5) = 2$ was proved in Ref. [31] by another approach. We have two remarks: First, for any four-dimensional pure state, Eq. (C9) is equivalent to

$$\langle\mathbb{I}X\rangle^2 + \langle\mathbb{I}Z\rangle^2 + \langle XY\rangle^2 + \langle YY\rangle^2 + \langle ZY\rangle^2 = 1. \tag{C10}$$

By permuting X, Y, Z, and the parties, we can obtain other equalities. Second, the standard SAUR of G_{10} cannot be generated by the construction in Lemma 2, since there is no operator anticommuting with $X\mathbb{I}, Y\mathbb{I}, Z\mathbb{I}$ at the same time; meanwhile, the dimension of the linear span of all the operators in this standard SAUR is 10.

Theorem 18. For a given graph G that can be divided into two subgraphs G_1 and G_2 where all vertices in G_1 are connected with all vertices in G_2, then $\beta(G) = \max\{\beta(G_1), \beta(G_2)\}$.

Proof. For a given SAUR of G, we label the operators for G_1 as $\{A_i\}$ and the operators for G_2 as $\{B_j\}$.

On the one hand, for any state ρ (for convenience, we omit the state ρ in the mean value), we have

$$\begin{aligned}\sum_i \langle A_i\rangle^2 + \sum_j \langle B_j\rangle^2 &= \max_{x,y}\left[\left\langle\sum_i x_i A_i\right\rangle^2 + \left\langle\sum_j y_j B_j\right\rangle^2\right] \\ &= \max_{x,y,t}\left[\left\langle t_1\sum_i x_i A_i + t_2\sum_j y_j B_j\right\rangle^2\right] \\ &\leq \max_{x,y,t}\left\langle\left(t_1\sum_i x_i A_i + t_2\sum_j y_j B_j\right)^2\right\rangle,\end{aligned} \tag{C11}$$

where x, y, and t are unit real vectors.

By the definition of $\{A_i\}$ and $\{B_j\}$, we have

$$\begin{aligned}
&\max_{x,y,t}\left\langle\left(t_1\sum_i x_iA_i+t_2\sum_j y_jB_j\right)^2\right\rangle\\
&=\max_{x,y,t}\left[t_1^2\left\langle\left(\sum_i x_iA_i\right)^2\right\rangle+t_2^2\left\langle\left(\sum_j y_jB_j\right)^2\right\rangle\right]\\
&=\max_{x,y,t}\max\left\{\left\langle\left(\sum_i x_iA_i\right)^2\right\rangle,\left\langle\left(\sum_j y_jB_j\right)^2\right\rangle\right\}\\
&\le\max_{x,y,t}\max\{\beta(G_1),\beta(G_2)\}\\
&=\max\{\beta(G_1),\beta(G_2)\}.
\end{aligned}\tag{C12}$$

By definition,

$$\beta(G)=\max_{\rho,\{A_i\},\{B_j\}}\left[\sum_i\langle A_i\rangle_\rho^2+\sum_j\langle B_j\rangle_\rho^2\right],\tag{C13}$$

which implies that $\beta(G)\le\max\{\beta(G_1),\beta(G_2)\}$.

On the other hand, $\beta(G)\ge\max\{\beta(G_1),\beta(G_2)\}$, which completes the proof. ■

Corollary 4. If we add one new vertex to a graph G and this results in a graph G' where the new vertex is connected to all vertices in G, then $\beta(G')=\beta(G)$.

Theorem 19. For a given graph G that can be divided into two subgraphs G_1 and G_2 where any vertex in G_1 is disconnected from any vertex in G_2, $\beta(G)=\beta(G_1)+\beta(G_2)$.

Proof. Without loss of generality, we assume that the state ρ and the SAUR $\{A_i\}$ result in $\beta(G_1)$, and that the state σ and the SAUR $\{B_j\}$ result in $\beta(G_2)$. Then $\{A_i\otimes\mathbb{I}_B\}\cup\{\mathbb{I}_A\otimes B_j\}$ is a SAUR of G. Direct calculation shows that

$$\sum_i\langle A_i\otimes\mathbb{I}\rangle_{\rho\otimes\sigma}^2+\sum_j\langle\mathbb{I}\otimes B_j\rangle_{\rho\otimes\sigma}^2=\beta(G_1)+\beta(G_2).\tag{C14}$$

Besides, for any SAUR $\{\tilde{A}_i\}\cup\{\tilde{B}_j\}$ of G and any state τ, we have

$$\begin{aligned}
\sum_i\langle\tilde{A}_i\rangle_\tau^2+\sum_j\langle\tilde{B}_j\rangle_\tau^2&\le\max_{\rho,\{A_i\}}\sum_i\langle A_i\rangle_\rho^2+\max_{\sigma,\{B_j\}}\sum_j\langle B_j\rangle_\sigma^2\\
&=\beta(G_1)+\beta(G_2).
\end{aligned}\tag{C15}$$

In total, we have $\beta(G)=\beta(G_1)+\beta(G_2)$ by definition. ■

For two given graphs G_1 and G_2, we denote by $G_1[G_2]$ their lexicographic product, whose vertex set is the Cartesian product of the graphs' vertex sets and then $(i_1,j_1)\sim(i_2,j_2)$ if $i_1\sim i_2$, or $j_1\sim j_2$ when $i_1=i_2$.

Theorem 20. For two given graphs G_1 and G_2, $\beta(G)$ is multiplicative under the lexicographic product: $\beta(G_1[G_2])=\beta(G_1)\beta(G_2)$.

Proof. Denote by $\{A_{ij}\}$ any SAUR of $G=G_1[G_2]$, where A_{ij} represents the vertex in G that corresponds to i in G_1 and j in G_2. Denote $\bar{A}_i=\sum_j x_{ij}A_{ij}/\lambda_i$, where $\{x_{ij}\}_j$ is the normalized vector of $\{\langle A_{ij}\rangle\}_j$ and λ_i is the maximal eigenvalue of $\sum_j x_{ij}A_{ij}$. We remark that $\{\bar{A}_i\}\in\mathcal{S}_{ac}^{\le}(G_1)$ and that $\{A_{ij}\}_j\in\mathcal{S}_{ac}(G_2)$ for all i.

By definition,

$$\begin{aligned}
\beta(G)&=\max_{\rho,\{A_{ij}\}\in\mathcal{S}_{ac}(G)}\sum_i\sum_j\langle A_{ij}\rangle_\rho^2\\
&=\max_{\rho,\{A_{ij}\}\in\mathcal{S}_{ac}(G)}\sum_i\left\langle\sum_j x_{ij}A_{ij}\right\rangle_\rho^2\\
&=\max_{\rho,\{A_{ij}\}\in\mathcal{S}_{ac}(G)}\sum_i\lambda_i^2\langle\bar{A}_i\rangle_\rho^2\\
&\le\beta(G_2)\max_{\rho,\{A_i\}\in\mathcal{S}_{ac}^{\le}(G_1)}\sum_i\langle A_i\rangle_\rho^2\\
&=\beta(G_2)\beta(G_1),
\end{aligned}\tag{C16}$$

where the inequality in the fourth line is from

$$\lambda_i^2=\max_\rho\left\langle\sum_j x_{ij}A_{ij}\right\rangle_\rho^2\le\beta(G_2)\tag{C17}$$

and the last equality is proven in Sec. VI.

On the other hand, without loss of generality, we assume that the state ρ and the SAUR $\{A_i\}$ result in $\beta(G_1)$ and that the state σ and the SAUR $\{B_j\}$ result in $\beta(G_2)$. Denote

$$A_{ij}=A_i\otimes\left[\bigotimes_{k\in G_1}B_j^{\delta_{ik}}\right],\tag{C18}$$

where $\delta_{ik}=1$ if $k=i$, otherwise $\delta_{ik}=0$. By construction, $\{A_{ij}\}\in\mathcal{S}(G)$. Let $\tau:=\rho\otimes\sigma^{\otimes n_1}$, where n_1 is the number of vertices in G_1. Then we have

$$\sum_{ij}\langle A_{ij}\rangle_\tau^2=\sum_{ij}\langle A_i\rangle_\rho^2\langle B_j\rangle_\sigma^2=\beta(G_1)\beta(G_2),\tag{C19}$$

concluding the proof. ■

For any large graph with decomposition into small graphs with known β numbers through the two addition operations and the lexicographic product, its exact β number can be obtained. For example, if we take the lexicographic product of five $\bar{C}_7$'s, i.e., $G = \bar{C}_7^{[\,]5}$, then $\beta(G) = \beta(\bar{C}_7)^5 \approx 40.2452$. However, $\alpha(G) = \alpha(\bar{C}_7)^5 = 32$ and $\vartheta(G) = \vartheta(\bar{C}_7)^5 \approx 41.8144$ since those two parameters are also multiplicative under the lexicographic product [48–50]. Hence, the integer parts of $\beta(G)$, $\alpha(G)$, and $\vartheta(G)$ can be all different. This closes the open question in Ref. [31] with the answer that there are indeed graphs with a β number strictly larger than the independence number, and the gap between them can even be large.

The removal of one edge is also one basic graph operation, which can relate different graph products. One important property shared by the independence number and the Lovász number is that they do not decrease under edge removal. However, this does not hold for the β number. Here we take $\bar{C}_7$ and its subgraph G_7 (see Fig. 4) as an example.

Theorem 21. $\beta(G_7) = 2 < \beta(\bar{C}_7)$.

Proof. Note that G_7 is isomorphic to an induced subgraph of $C_5[K_2]$, where K_2 is just one edge. Thus,

$$\beta(G_7) \leq \beta(C_5)\beta(K_2) = 2. \tag{C20}$$

On the other hand, $\beta(G_7) \geq \alpha(G_7) = 2$, which completes the proof. ■

Although the β number is between the independence number and the Lovász number, its behavior under edge removal is rather strange. Nevertheless, the β number does not increase under vertex removal, and the same is true for the independence number and the Lovász number. More explicitly, $\beta(G') \leq \beta(G)$ if G' is an induced subgraph of G.

The tensor product of systems is often used in quantum mechanics. Denote by G the anticommutativity and commutativity graph corresponding to the tensor product of the SAURs of G_1 and G_2. We can directly verify that G is the XOR product of G_1 and G_2, i.e., $(i_1,j_1) \sim (i_2,j_2)$ if and only if only one of $i_1 \sim i_2$ and $j_1 \sim j_2$ holds. In this case, denote $G = G_1 \times G_2$.

Theorem 22. For two given graphs G_1 and G_2, $\beta(G_1 \times G_2) \geq \beta(G_1)\beta(G_2)$.

Proof. Denote by $\{A_i\}$ and $\{B_j\}$ the standard SAUR of G_1 and the standard SAUR of G_2, respectively. Then we know that

$$q(\{A_i\}) = \beta(G_1), q\left(\{B_j\}\right) = \beta(G_2). \tag{C21}$$

Hence,

$$\begin{aligned}\beta(G_1 \times G_2) &\geq q\left(\{A_i \otimes B_j\}\right) \\ &\geq \max_{\rho_1\otimes\rho_2} \sum_{ij} \langle A_i \otimes B_j\rangle^2_{\rho_1\otimes\rho_2} \\ &= \beta(G_1)\beta(G_2),\end{aligned} \tag{C22}$$

since $\{A_i \otimes B_j\}_{ij}$ is a SAUR of $G_1 \times G_2$. ■

For a perfect graph G, we know that $\alpha(G) = \vartheta(G) = \alpha^\star(G)$, which implies that $\alpha(G) = \beta(G) = \vartheta(G) = \alpha^\star(G)$. For imperfect graphs, odd cycles and odd anticycles are basic building blocks. To continue, we make the following claim.

Theorem 23.

$$\max_\rho \left[\langle \mathbb{I}Y\rangle^2_\rho + \langle XX\rangle^2_\rho + \langle ZZ\rangle^2_\rho - \langle YY\rangle^2_\rho\right] = 1. \tag{C23}$$

Proof. It is enough to show that the maximum of the following SDP is 1, as a relaxation of the original theorem:

$$\begin{aligned} l = \max_\gamma \operatorname{Tr}\gamma W& \\ \text{such that } \operatorname{Tr} A_0\gamma = 1,\ \gamma \succeq 0,& \\ \operatorname{Tr} A_i\gamma \geq 0,\ i = 1,2,3,&\end{aligned} \tag{C24}$$

where $W = \mathbb{I}Y\mathbb{I}Y + XXXX + ZZZZ - YYYY$, $A_0 = \mathbb{I}\mathbb{I}\mathbb{I}\mathbb{I}$, $A_1 = XZXZ$, $A_2 = Y\mathbb{I}Y\mathbb{I}$, and $A_3 = ZXZX$.

Then the dual SDP is

$$\begin{aligned} l' = \min y_0& \\ \text{such that } \sum_{i=0}^3 y_iA_i - W \succeq 0,& \\ y_i \leq 0,\ i = 1,2,3.&\end{aligned} \tag{C25}$$

Since the case that $y_0 = 1$ and $y_i = -1$ for $i = 1,2,3$ is a feasible solution, we know that $l \leq l' \leq 1$. However, by taking $\rho = |\Psi^+\rangle\langle\Psi^+|$ with $|\Psi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ in Eq. (C23), we have $l \geq 1$. Consequently, $l = 1$. ■

It is known that $l = 1$ if we consider only the state in the form $\rho = (\mathbb{I} + xXX + yYY + zZZ)/4$, for which $\langle \mathbb{I}Y\rangle_\rho = 0$ [59]. Hence, our result generalizes the known result, which is often considered in quantum correlations such as discord [59].

By considering the relation between the standard SAUR of different odd cycles, we have the following lemma.

Lemma 3. $\beta(C_{2n+3}) - \beta(C_{2n+1}) \le 1$.

Proof. For convenience, we label the vertices of C_{2k+1} in such a way that

$$1 \sim 3 \sim \cdots \sim 2k+1 \sim 2(k-1) \sim \cdots \sim 2, \tag{C26}$$

where $k = n, n+1$.

The proof is based on the observation that the standard SAUR $\{S'_i\}_{i=1}^{2n+3}$ of C_{2n+3} can be constructed as follows:

$$\begin{aligned} &S'_i = S_i \mathbb{I}_2 \text{ for all } i = 1, \ldots, 2n, \\ &S'_{2n+1} = \mathbb{I}_{2^{n-1}} XX, \quad S'_{2n+2} = \mathbb{I}_{2^{n-1}} ZZ, \\ &S'_{2n+3} = \mathbb{I}_{2^n} Y, \end{aligned} \tag{C27}$$

where $\{S_i\}_{i=1}^{2n} \cup \{\mathbb{I}_{2^{n-1}} Y\}$ is the standard SAUR of C_{2n+1}.

If we denote $S''_{2n+1} = \mathbb{I}_{2^{n-1}} YY$, we have

$$\begin{aligned} \beta(C_{2n+3}) &= \max_{\sigma'} \left[\sum_{i=1}^{2n} \langle S'_i \rangle_{\sigma'}^2 + \sum_{i=2n+1}^{2n+3} \langle S'_i \rangle_{\sigma'}^2 \right] \\ &= \max_{\sigma'} \left[\left(\sum_{i=1}^{2n} \langle S'_i \rangle_{\sigma'}^2 + \langle S''_{2n+1} \rangle_{\sigma'}^2 \right) \right. \\ &\quad \left. + \left(\sum_{i=2n+1}^{2n+3} \langle S'_i \rangle_{\sigma'}^2 - \langle S''_{2n+1} \rangle_{\sigma'}^2 \right) \right] \\ &\le \beta(C_{2n+1}) + 1, \end{aligned} \tag{C28}$$

where the last inequality is from the fact that $\{S'_i\}_{i=1}^{2n} \cup \{S''_{2n+1}\}$ is one SAUR of C_{2n+1} and Theorem 23. ■

Since $\alpha(C_{2n+1}) = n$ and $\beta(C_5) = \alpha(C_5) = 2$, Theorem 23 and Lemma 3 lead to the following theorem.

Theorem 24. $\overline{\mathcal{Q}}\,(\mathcal{S}_{ac}(C_m)) = \text{STAB}(C_m)$.

Proof. Since C_m is a perfect graph when m is an even number, the fact that $\text{STAB}(C_m) = \text{TH}(C_m)$ implies that $\overline{\mathcal{Q}}\,(\mathcal{S}_{ac}(C_m)) = \text{STAB}(C_m)$.

When $m = 2n+1$ is an odd number, Theorem 23 and Lemma 3 result in the fact that $\beta(C_{2n+1}) = \alpha(C_{2n+1})$. Consequently, this implies that $\overline{\mathcal{Q}}\,(\mathcal{S}_{ac}(C_{2n+1})) = \text{STAB}\,(C_{2n+1})$, since the only nontrivial facet of $\text{STAB}(C_{2n+1})$ has the norm vector $(1, \ldots, 1)$ [60]. ■

Theorem 25. $\mathcal{Q}\left(\mathcal{S}_a^{\le}(G)\right) = \mathcal{Q}\,(\mathcal{S}_a G) = \text{TH}(G)$.

Proof. Note that $\text{TH}(G) \subseteq \mathcal{Q}\,(\mathcal{S}_a(G)) \subseteq \mathcal{Q}\left(\mathcal{S}_a^{\le} G\right)$. Hence, it is sufficient to prove $\mathcal{Q}\left(\mathcal{S}_a^{\le} G\right) \subseteq \text{TH}(G)$ or, equivalently, $q\left(\mathcal{S}_a^{\le}(G), w\right) \le \vartheta(G, w)$ for any nonnegative weight vector w.

For a given SARA $\{A_i\}$ and a state ρ, denote $\omega_i = \text{Tr}\, A_i^2 \rho$. The fact that $A_i^2 \le \mathbb{I}$ leads to $\omega_i \le 1$. Then [61]

$$\sum_i w_i \langle A_i \rangle_\rho^2 \le \lambda(\mathcal{A}), \tag{C29}$$

where $\mathcal{A}$ is a matrix with (i,j)th element $\sqrt{w_i w_j}\,\langle \{A_i, A_j\} \rangle /2$. Thus, the ith diagonal term of $\mathcal{A}$ is $w_i \omega_i$, and the (i,j)th element is 0 if $i \sim j$. Denote $w' = (w_i \omega_i)$. Note that [44]

$$\vartheta(G, w') = \max_{\mathcal{B}} \lambda(\mathcal{B}),$$
$$\text{subject to } \mathcal{B}_{ij} = 0 \text{ if } i \sim j, \tag{C30}$$

$$\mathcal{B}_{ii} = w'_i, \tag{C31}$$

$$\mathcal{B} \ge 0. \tag{C32}$$

Thus, by definition, we have $\lambda(\mathcal{A}) \le \vartheta(G, w')$. Meanwhile, $\vartheta(G, w') \le \vartheta(G, w)$ since $w'_i \le w_i$ for each i. ■

Lemma 4. For a given graph G and one SAR $\{A_i\}$ of it, there is a unitary U such that

$$U A_i U^\dagger = \oplus_{t=1}^T A_i^{(t)}, \quad [A_i^{(t)}]^2 = [\lambda_i^{(t)}]^2 \mathbb{I}_{d_t}, \tag{C33}$$

where $\{\lambda_i^{(t)}\}$ are singular values of A_i. Besides, $\{A_i^{(t)}\}$ is a SAR of G for any $t = 1, \ldots, T$.

Proof. We note that $[A_i^2, A_j] = 0$ and $[A_i^2, A_j^2] = 0$ for any pair (i,j). Hence, there is a unitary U to diagonalize all the A_i^2's simultaneously. By ordering the diagonal terms properly, we have the decomposition

$$U A_i^2 U^\dagger = \oplus_{t=1}^T [\lambda_i^{(t)}]^2 \mathbb{I}_{d_t}. \tag{C34}$$

Denote by $\{\langle u|\}$ the rows of U. Then by choosing $|u\rangle, |v\rangle$ such that $A_i^2 |u\rangle = [\lambda_i^{(t)}]^2 |u\rangle$ and $A_i^2 |v\rangle = [\lambda_i^{(l)}]^2 |v\rangle$, we have

$$\langle u| A_i^2 A_j |v\rangle = [\lambda_i^t]^2 \langle u| A_j |v\rangle = \langle u| A_j A_i^2 |v\rangle = [\lambda_i^l]^2 \langle u| A_j |v\rangle. \tag{C35}$$

Hence, $\langle u| A_j |v\rangle = 0$ whenever $\lambda_i^{(t)} \ne \lambda_i^{(l)}$. This leads to the desired decomposition as in Eq. (C33). ■

Lemma 5. For any given $\{S_i\} \in \mathcal{S}_{ac}(G)$, state ρ, and weight vector w where $|w_i| \le 1$, there exists $\{P_i\} \in \mathcal{S}_{ac}(G)$ and state τ such that $\langle P_i \rangle_\tau = w_i \langle S_i \rangle_\rho$.

Proof. Denote

$$P_i = S_i \otimes (\otimes_j Z(w_i)^{\delta_{ij}}), \quad \tau = \rho \otimes (|+\rangle\langle+|)^{\otimes n}, \tag{C36}$$

where $Z(w) = wX + \sqrt{1-w^2} Z$ for $t \in [-1, 1]$, $\delta_{ij} = 1$ if $i = j$ and otherwise $\delta_{ij} = 0$, and n is the number of vertices in G. Direct calculation concludes the proof. ■

Lemma 5 also implies that $\mathcal{Q}(\mathcal{S}_{ac}(G))$ is star-convex.

Theorem 26. $\mathcal{Q}\left(\mathcal{S}_{ac}^{\leq}(G)\right) = \mathcal{Q}(\mathcal{S}_{ac}G)$.

Proof. To prove this theorem is equivalent to prove that for any given $\{S_i\} \in \mathcal{S}_{ac}^{\leq}(G)$ and state ρ, there is a $\{P_i\} \in \mathcal{S}_{ac}(G)$ and state τ such that $\langle S_i \rangle_\rho = \langle P_i \rangle_\tau$. Without loss of generality, we assume that $S_i = \oplus_{t=1}^{T} S_i^{(t)}$, where $S_i^{(t)}$ acts on $\mathcal{H}^{(t)}$. A direct calculation shows that

$$\langle S_i \rangle_\rho = \sum_t p_t \left\langle S_i^{(t)} \right\rangle_{\rho_t}, \tag{C37}$$

where ρ_t is the block of ρ in $\mathcal{H}^{(t)}$ up to the normalization coefficient p_t.

From Lemma 5, we know that there exists $\{P_i^{(t)}\} \in \mathcal{S}_{ac}(G)$ and state τ_t such that $\left\langle S_i^{(t)} \right\rangle_{\rho_t} = \left\langle P_i^{(t)} \right\rangle_{\tau_t}$. Consequently,

$$\langle S_i \rangle_\rho = \sum_t p_t \left\langle P_i^{(t)} \right\rangle_{\tau_t}. \tag{C38}$$

If we denote $P_i = \oplus_t P_i^{(t)}$ and $\tau = \oplus_t p_t \tau_t$, we have $\{P_i\} \in \mathcal{S}_{ac}(G)$ and τ is a quantum state. Equation (C38) implies that $\langle S_i \rangle_\rho = \langle P_i \rangle_\tau$. ■

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