Contextuality with Pauli observables in cycle scenarios

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Abstract

Contextuality is a fundamental, rigorous marker of non-classicality exhibited by quantum theory, which has been shown to be a resource for quantum computational advantage in a variety of settings. Such results often boil down to contextuality relative to Pauli observables. In this work, we initiate a systematic study of Pauli contextuality by considering scenarios where the measurement compatibility structure is described by a cycle. For any n, we show that the maximum size of a cycle realizable by n-qubit Pauli observables is upper bounded by $3n$. We then prove that no such k-cycle Pauli realization for $k > 4$ can witness contextuality (on any quantum state), whereas for $k = 4$ every Pauli realization exhibits contextuality, attaining the quantum bound for any noncontextuality inequality on some pure state. Finally, we discuss the effect of cycles on the presence of contextuality in arbitrary Pauli scenarios in light of Vorob'ev's theorem, which requires the presence of cycles for a scenario to witness contextuality.

1 Introduction

1.1 Motivation

Contextuality is a fundamental, rigorous marker of non-classicality exhibited by quantum theory. It seems natural to expect this non-classical feature to play a vital role as a resource for quantum computational advantage. Indeed, many such links have been unveiled recently, and many such results boil down to contextuality relative to Pauli observables. For example, Howard et al. [6] showed that contextuality is a necessary resource for universal quantum computation via magic state distillation, while Raussendorf [13] proved that the measurement-based quantum computation model (with mod 2 classical control) cannot compute nonlinear Boolean functions without the presence of contextuality. Both these results involve contextuality with respect to (qudit or qubit) Pauli observables only. Indeed, Pauli measurements play a central role in many models of quantum computation, relevant to both near-term and fault-tolerant settings. A recently proposed universal model called Pauli-based computation model involves sequential measurement of adaptively chosen commuting Pauli observables on an initially prepared magic state [4]. On the other hand, hybrid algorithms like variational quantum eigensolvers (VQEs), which are considered strong candidates for witnessing practical quantum advantage in NISQ devices, also involve measurements of Pauli observables in each iteration. Focusing on the measurement part of VQE, Kirby and Love [7] defined a contextuality test on VQE instances. Subsequently [8], they showed that the classical simulation of noncontextual VQEs is *only* an NP-complete problem, i.e. it is at worst classically hard (as opposed to quantumly hard, represented by the QMA complexity class). This ubiquity of Pauli observables makes it crucial to extract as much as we can about their contextuality aspects.

Indeed, Pauli observables have also been studied in quantum foundations and, specifically in the qubit case, used to provide especially simple and appealing proofs of contextuality, namely proofs of (state-dependent or state-independent) strong contextuality, with a powerful logical flavour. Two of the simplest such instances of contextuality are provided by the Peres–Mermin square [11] and the Mermin star [10]. Introduced as enormous simplifications of the Kochen–Specker 117-vector construction [9], they consist of particular arrangements of nine (resp. ten) two-qubit Pauli observables that admit no non-contextual value assignment consistent with the support of the empirically observable probabilities (on joint outcomes of contexts of compatible, i.e. commuting, observables), for *any* quantum state.

The contextuality test for VQE instances proposed in [7] concerns precisely such state-independent contextuality. The instances considered in that work are given by Hamiltonians expressed in Pauli decomposition, i.e. as a linear combination of operators from the n-qubit Pauli group $\mathcal{P}_n$. Starting from the set $S \subseteq \mathcal{P}_n$ of Paulis appearing in such a decomposition, it considers its closure $\bar{S}$ under products of commuting elements.[1]The instance is deemed to be contextual if $\bar{S}$ exhibits state-independent strong contextuality (like the above-mentioned square and star). The authors also provide a necessary and sufficient condition on the set S for this to happen. The initial motivation for the present work comes from noticing the following caveat in this analysis. The VQE algorithm performs only the measurements in S, not those in $\bar{S}$. As such, in a classical simulation, it suffices to reproduce the statistics of these measurements on certain quantum states, regardless of whether they could be consistently extended to encompass $\bar{S}$. A more refined classicality analysis would thus focus on the (weak) contextuality of the correlations realizable by the measurements of S alone on some quantum state.

While strong contextuality relative to n-qubit Paulis has been extensively studied, from the state-independent proofs mentioned above to state-independent arguments such as GHZ or, more generally, All-versus-Nothing arguments [2, 1], probabilistic (a.k.a. weak) contextuality has received little attention. In this work, we initiate a systematic study of the following question, prompted by the discussion above: *given a set S of n-qubit Pauli operators, when does it directly witness contextuality?*

One way to approach this question is to take the compatibility graph of Pauli operators in S and treat it as an abstract measurement scenario. One can then derive all the noncontextuality inequalities for this scenario and test whether the given Pauli realisation can violate any of them. A major bottleneck, however, is that finding all the noncontextuality inequalities for an arbitrary scenario encoded as a compatibility graph is an NP-complete problem. Hence, as a way to get a handle on the general problem, we start by considering a specific, simple class of measurement scenarios: those where the measurement compatibility structure is given by a cycle graph C_k. Two main reasons inform this choice:

1. All the noncontextuality inequalities for these scenarios have been explicitly characterised in [3]. In fact, these are the only fully characterised non-Bell-type scenarios to date.
2. Vorob'ev's theorem [14] theorem, phrased in terms of compatibility graphs, requires the presence of at least one cycle of size $k \geq 4$ as an *induced* subgraph for a scenario to admit any contextual correlations. Cycle graphs are thus the simplest measurement scenarios that may exhibit contextuality.

1.2 Contributions

Focusing on cycle scenarios, we pose the following questions, which we address in this work.

Question A. Which cycle scenarios are realizable[2]by n-qubit Pauli operators (for each fixed n)?

Question B. Which Pauli cycles witness contextuality on some quantum state?

Partially addressing Question A, we prove an upper bound on the maximum size of realizable cycles for each number of qubits.

Theorem 1. *If a k-cycle is realizable by n-qubit Pauli operators then $k \leq 3n$.*

We also performed an exhaustive computational search for small n and k, concluding that: (i) the bound in Theorem 1 is not tight in general; and (ii) for fixed n, some values of k are 'skipped', e.g. there is a 9-cycle of 3-qubit Paulis, but no 8-cycle. These observations raise the question of whether our methods can be pushed further in order to lower the upper bound and/or exclude such exceptions.

Turning our attention to Question B, we manage to provide a complete answer, which splits into two extreme cases: for $k > 4$, no k-cycle of Paulis can witness contextuality, while for $k = 4$ every Pauli realisation not only exhibits contextuality but can even attain the quantum bound for all noncontextuality inequalities.

Theorem 2. *Let $\{P_i\}_{i=0}^{k-1}$ be a Pauli realisation of the k-cycle graph for some $k > 4$. Then, for any quantum state, the corresponding empirical model (a.k.a. correlation) is noncontextual.*

Theorem 3. *Let $\{P_i\}_{i=0}^{3}$ be any Pauli realisation of the 4-cycle graph. Then, for any noncontextuality inequality of the 4-cycle scenario, there is a pure quantum state that violates it, moreover attaining the quantum bound.*

[1] $\bar{S}$ is the partial Abelian group (in the same sense of partial Boolean algebra) generated by S *within* $\mathcal{P}_n$; we refer to upcoming work for more about this perspective.

[2] An n-qubit Pauli realization of a graph $G = (V, E)$ is an assignment $P \colon V \to \mathcal{P}_n$ of n-qubit Pauli operators to vertices of the graph such that $P(v)$ and $P(w)$ commute if and only if $v = w$ or $\{v, w\} \in E$. When G is a cycle of size at least 4 a realization must necessarily be injective. Hence, it amounts to an isomorphic copy of G as an induced subgraph of the compatibility graph of $\mathcal{P}_n$.

In light of Vorob'ev's theorem, which requires the presence of cycles for a graph to exhibit contextuality, one wonders whether Theorems 2 and 3 provide a clue for a complete characterisation beyond cycle scenarios.

Question C. Is an induced 4-cycle necessary and sufficient for contextuality in arbitrary Pauli scenarios?

It turns out that the answer is no: while it is clearly sufficient given Theorems 3, it is not necessary. We exhibit an example of a graph with a Pauli realization that admits a contextual model even though none of its induced cycles does, as they have size greater than 4.

1.3 Methods

We now provide a brief outline of the proofs of our results, to give a flavour of the key methods and ideas used. Full details can be found in the corresponding sections.

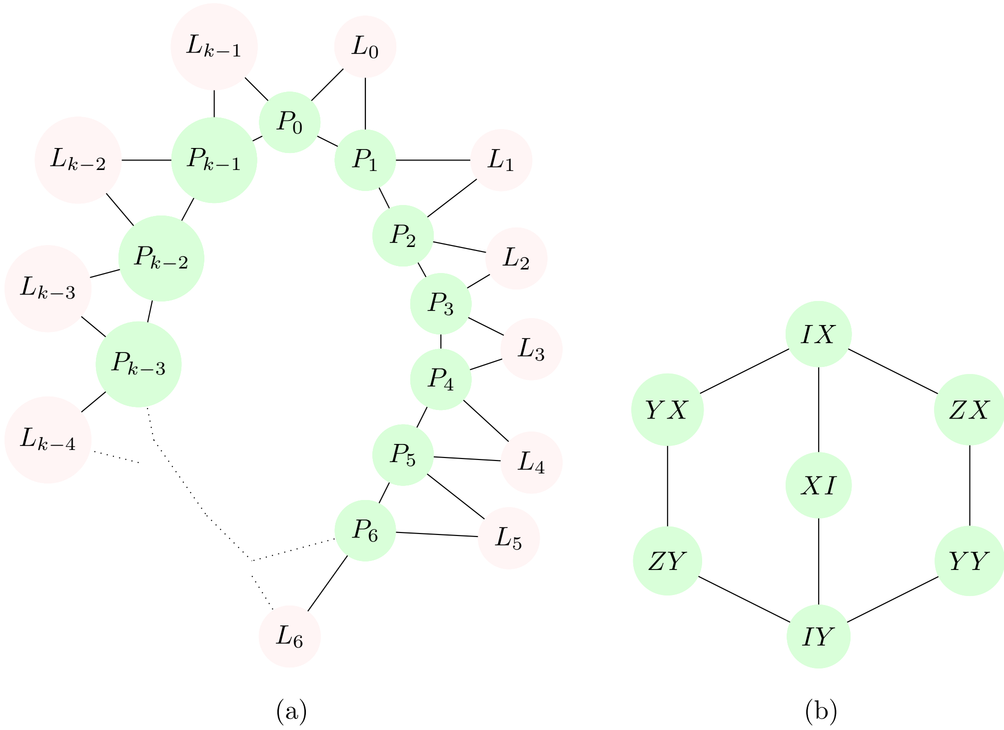

Figure 1: (a) Construction used to answer Questions A and B: Arbitrary Pauli k-cycle (green) and the constructed edge Paulis $L_i = P_i P_{i\oplus 1}$ (pink). Each edge Pauli commutes with all other edge Paulis except the two nearest neighbours on both sides. (b) Example negatively answering Question C: Pauli realization of two conjoined 5-cycles, which violates a non-cycle noncontextuality inequality.

Question A For the computational search, we ran (induced) subgraph isomorphism tests within the compatibility graphs of $\mathcal{P}_n$ for each n. To prove the theorem, we start off with an arbitrary Pauli realisation $\{P_i\}_{i=0}^{k}$ of a cycle and extend it through the construction depicted in Figure 1-(a). For each edge in the cycle, we add an "edge" Pauli, $L_i = P_i P_{i\oplus 1}$.[3] Crucially, whether each of these L_i commutes or anti-commutes with the original cycle Paulis and with the other L_i can be determined by a general rule, which does not depend on the concrete cycle Paulis we started from: namely, a Pauli Q commutes with L_i if and only if it commutes with both P_i and $P_{i\oplus 1}$ or with neither. In other words, the neighbourhood of L_i in the compatibility graph of Paulis is the exclusive disjunction between those of P_i and of $P_{i\oplus 1}$. We use this commutativity structure and the fact that any maximal stabilizer subgroup is generated by n independent, pairwise commuting Paulis to derive the upper bound of $3n$ (Theorem 1). Full details can be found in section 2.

[3]These new Paulis are not taken to be part of the contextuality scenario; they are simply a device to help derive a contradiction.

Question B All noncontextuality inequalities in a k-cycle scenario [3] have the form:

$$\sum_{i=0}^{k-1} \gamma_i \langle A_i A_{i\oplus 1}\rangle \overset{NCHV}{\leq} k-2, \qquad \text{for } \gamma_i \in \{-1,+1\} \text{ with } \prod_{i=0}^{k-1} \gamma_i = -1.$$

where $\{A_i\}_{i=0}^{k-1}$ are the measurements labelling each vertex. For a Pauli realization, each term of the sum on the left corresponds to an edge Pauli L_i, again as in Figure 1-(a), so that the quantity being bounded is the expectation value of the operator $N := \sum_{i=0}^{k-1} \gamma_i L_i$. Squaring N and using simple algebra and the commutativity properties of edge Paulis, we conclude:

- for $k > 4$, that $\langle N^2\rangle \leq k^2 - 4k < (k-2)^2$, from which Theorem 2 follows;
- for $k = 4$, that $N^2 = 4(I + \gamma_1\gamma_3 P_0P_1P_2P_3)$, where $\gamma_1\gamma_3 \in \{-1,+1\}$, so that any $\gamma_1\gamma_3$-eigenstate $|\psi\rangle$ of $P_0P_1P_2P_3$ (itself a Pauli) yields $\langle N^2\rangle_{|\psi\rangle} = 8$ and $\langle N\rangle_{|\psi\rangle} = \pm 2\sqrt{2}$.

Details of these derivations can be found in section 3. In particular, the $k = 4$ case is analysed in section 3.1, and the $k > 4$ in sections 3.2 (illustration of method with $k = 5$) and 3.3 (general case).

Question C Figure 1-(b) shows a Pauli realization of a graph consisting of two 5-cycles glued along two edges. We found new non-cycle inequalities for this scenario using the PORTA package [5]. One such inequality is written, in operator-theoretic form and for this particular Pauli realization, as

$$-(ZI + XZ + YI + XY + YI) + ZI - (IY + XI + ZY + YX) \leq 4I.$$

The maximum eigenvalue of the operator sum on the left-hand side turns out to be $4.2716 > 4$, implying that the inequality is violated for some (eigen)state. This happens despite the fact that individual cycles in the scenario cannot exhibit contextuality by themselves, offering a counterexample to the conjecture implicit in Question C. One may conclude that while the presence of cycles in arbitrary scenarios is required to impede Vorob'ev's inductive construction of a probability distribution on joint outcomes for all measurements, it is not the case that every instance of contextuality can be witnessed in a single cycle. This last question is address in section 4.

2 Pauli operators on cycles

To answer what k-cycles are Pauli realizable, for a given n, we developed on our guiding intuition that constructing edge Pauli operators over a Pauli realized cycle must enforce constraints which might be leveraged to derive an upper bound on the allowed maximal cycle size. Turns out that the intuition works.

But before the details, we start with some notational clarification: $\mathcal{P}_\mathbf{n}$ will denote ± 1 multiples of n-qubit Pauli operators. $\mathcal{M}$ denotes the set of Pauli operators realizing a cycle, $C_\mathcal{M}$ denotes the corresponding cycle graph with Pauli labellings from $\mathcal{M}$. $\mathcal{L}$ contains all the edge Pauli operators and $C_{\mathcal{M},\mathcal{L}}$ denotes the whole graph containing the edge Paulis appended to $C_\mathcal{M}$.

The definition of cycle imposes some constraints like (i) Forbidden Edge Paulis (ii) Commutativity structure within $C_{\mathcal{M},\mathcal{L}}$. Both are explained below. Understanding these constraints would then set us up for the proof for upper bound on realizable k-cycles.

We also emphasize that all throughout the following proofs we keep making use of the following properties of Paulis in $\mathcal{P}_\mathbf{n}$: (i) self-Inverse/Idempotent (ii) product of two commuting elements lies within $\mathcal{P}_\mathbf{n}$ (iii) two Paulis either commute or anti-commute.

2.1 Forbidden Edge Paulis

- No Edge Pauli can be the same as any of the cycle Paulis constituting it : $L_i = P_iP_{i\oplus 1}$ and $L_i \neq \pm P_i$ because if $L_i = \pm P_i \implies P_{i\oplus 1} = \pm I$. This means $P_{i\oplus 1}$ has to commute with all cycle Paulis too, which is forbidden since cycle Paulis can ONLY commute with the neighbouring Paulis in the cycle.
- Edge Pauli can't also be equal to any other cycle Pauli i.e. $L_i = P_iP_{i\oplus 1} \neq \pm P_l$ where $l \in \{0, 1, 2, 3..., k-1\} \setminus \{i,\ i\oplus 1\}$ because if $L_i = \pm P_l$ and since $[L_i, P_i] = 0 \implies [P_i, P_l] = 0$ which means that atleast one cycle Pauli constituting the edge Pauli L_i commutes with a non-neighbouring Pauli P_l which is forbidden for a Pauli cycle, by definition.

Basically, these rules capture the idea that no cycle Pauli is a multiple of edge Pauli and vice versa.

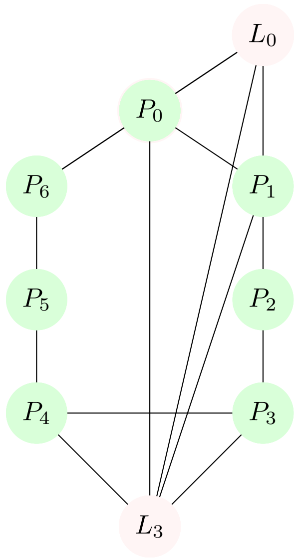

Figure 2: In the 2,7-cycle of Paulis (in green) we introduce two edge Paulis (in pink) $L_0 = P_0 P_1$; $L_3 = P_3 P_4$ and some more edges allowed by the four conditions obtained in section 4.1.

2.2 Commutativity structure of $\mathcal{C}_{\mathcal{M},\mathcal{L}}$

It is important to know the commutation relations between all Paulis existing within the graph $\mathcal{C}_{\mathcal{M},\mathcal{L}}$ i.e. beyond just the n,k-cycle ($\mathcal{C}_{\mathcal{M}}$): this constitutes commutation relations - within the set $\mathcal{L}$, summed up by 1-4 below & across $\mathcal{L}$ and $\mathcal{M}$, expressed in 5:

1. $\{L_i, L_{i\oplus 1}\} = 0$ and $\{L_i, L_{i\oplus(k-1)}\} = 0$. In words: no Pauli in $\mathcal{X}$ commutes with its nearest[4] edge Paulis.
2. For k > 4, $\{L_i, L_{i\oplus 2}\} = 0$ and $\{L_i, L_{i\oplus(k-2)}\} = 0$. In words: for k > 4, no Pauli in $\mathcal{L}$ commutes with its next-nearest edge Pauli.
3. Notice that for $k = 5$, for each edge Pauli, only the nearest and next-nearest edge Paulis exist. Hence the edge Pauli doesn't commute with any other edge Pauli.
4. For $k > 5$, $[L_i, L_j] = 0$ where $i \oplus 3 \leq j \leq i \oplus (k-3)$ i.e. for k > 5, Paulis in $\mathcal{L}$ commute with all other edge Paulis except the nearest and next-nearest ones.
5. $[L_i, P_l] = 0$ whenever $l \neq i \oplus (k-1)$ and $i \oplus 2$ i.e. each Pauli in $\mathcal{L}$ commutes with all cycle Paulis except the next-nearest ones indexed by $i \oplus (k-1)$ and $i \oplus 2$.

2.3 Allowed cycle sizes (k) for a given n

We start off by mentioning some observations coming from subgraph isomorphism test runs: for $n = 2$, we only observe cycles uptil size $k = 6$. For $n = 3$, all cycles of size 4 to 9 except the 8-cycle. For $n = 4$, no cycle after $k = 9$ exists. This means the 8-cycle is realized for the first time by $n = 4$ Pauli operators. To analytically investigate this observed upper bound, for the most general case, we start with case where $n = 2$ and assume that a 7-cycle exists. Fig. 1 serves as an illustration.

We assume that the cycle Paulis in figure 3 are 2-qubit Paulis i.e. $\mathcal{M} = \{P_i | P_i \in \mathcal{P}_2\}$. It is a well known result in stabilizer subtheory that a maximal stabilizer subgroup for n qubits has n independent generators. Here, n=2, now consider two independent commuting Paulis $\{P_0,\ L_0\}$ and the maximal subgroup, say $\mathcal{R}$, generated by them i.e. $\mathcal{R} \equiv \langle P_0, L_0 \rangle$. Since L_3 commutes with the generators in the maximal subgroup, hence $L_3 \in \mathcal{R}$ i.e. $L_3 = {P_0}^{\alpha} {L_0}^{\beta}$ where $\alpha, \beta \in \{0, 1\}$. Consider the four cases now:

- $\alpha = 0, \beta = 1 \implies L_3 = L_0$: This is forbidden because $[L_3, L_4] \neq 0$ but $[L_0, L_4] = 0$. These relations follow because of the conditions 2 and 3 respectively in section 5.1 .

[4] nearest w.r.t indices

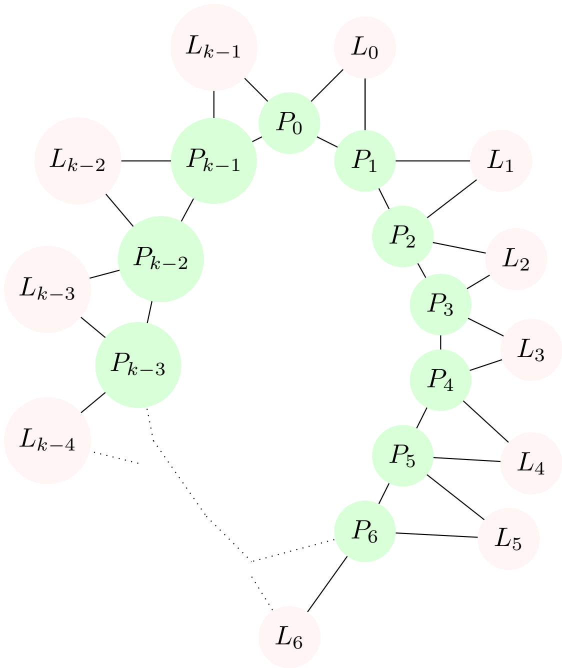

Figure 3: An arbitrary n,k-cycle (green) and edge Paulis $L_i = P_i P_{i\oplus 1}$ (pink), the dotted lines refers to the Paulis (including edge Paulis) not drawn but are part of the cycle.

- $\alpha = 1, \beta = 0 \implies L_3 = P_0$: This is forbidden because then $P_1 = I$ and the graph no more remains the 7-cycle.
- $\alpha = 0, \beta = 0 \implies L_3 = I$: This is forbidden because then $P_3 = P_4$ which means the graph no more remains the 7-cycle.
- $\alpha = 1, \beta = 1 \implies L_3 = P_0 L_0 = P_0 P_0 P_1 = P_1$: This is forbidden since it enforces the edges (P_3, P_1) and (P_4, P_1), hence again, the graph no more remains the 7-cycle.

This exhausts all the possibilities and hence a 2,7-cycle is prohibited. It can be trivially seen that the same argument will hold for any 2,k-cycle $\forall\ k \geq 7$.

Now, we generalise such cycle impossibility proof for any n:

Consider a generic Pauli n,k-cycle as in figure 4, with the edge Paulis included too i.e. the graph $\mathcal{C}_{\mathcal{M},\mathcal{L}}$. Collect together the following Paulis:

$$S \equiv \{P_0, L_0, L_3, L_6, ..., L_{k-6}, L_{k-3}\}$$

where by the conditions in section 4.1, Paulis in S pairwise commute:

1. in between any $L_l, L_k \in S$ there are atleast two edge Paulis in the graph (see figure 3) hence via condition 3 in section 4.1 both commute.
2. Each $L_k \in S$ commutes with P_0 via condition 4 above.

We now prove that Paulis in S are also independent[5]: First pick all the elements uptil L_i starting from P_0 from the n,k-cycle (in the clockwise sense of figure 3) from the set S i.e. $S_i \equiv \{P_0, L_0, L_3, L_6, ...L_{i-3}, L_i\}$. Consider the edge Pauli L_{i+1}. Via conditions 3 and 4 - L_{i+1} commutes with every element in $S_{i-1} = \{P_0, L_0, L_3, L_6, ..., L_{i-3}\}$. By construction L_i also commutes with every element in S_{i-1} and also via condition 1, $[L_i, L_{i+1}] \neq 0$. Then, $L_i \notin \langle P_0, L_0, L_3, L_6, ..., L_{i-3}\rangle$. Because if it did then $[L_i, L_{i+1}] = 0$ which we know can not hold true (via condition 1 derived in section 5.2). The above argument holds uptil any $L_i \in S$ except the last one i.e. L_{k-3} . Since for it, the Pauli $L_{(k-3)+1}$ does not commute with P_0, L_0

[5]independent means that no Pauli operator can be written as a product of other commuting Paulis

due to condition 4 and hence L_{k-3} cannot be guaranteed to be independent of the rest of the elements in S. So, we throw away this element from S. This proves that all Paulis in $S \setminus \{L_{k-3}\}$ are independent. We now update S:

$$S \equiv \{P_0, L_0, L_3, L_6, ..., L_{k-6}\}$$

Next, we prove the maximum size of cycle allowed for a given n. We know that for any given n, any maximal subgroup is generated by n independent, pairwise commuting Paulis. Therefore for the n,k-cycle i.e. when Paulis in S are n-qubit Paulis then $|S| \leq n$. From the pattern of edge Paulis in S (see figure 3), we can write S as $\{P_0, L_0, L_{3k}\}_{k=1}^{|S|-2}$. The case where $|S| = n$ i.e. $S = \{P_0, L_0, L_{3k}\}_{k=1}^{n-2} = \{P_0, L_0, L_3, ..., L_{k-6}\}$. This means that $L_{3(n-2)} = L_{k-6} \implies 3(n-2) = k-6 \implies k = 3n$. Hence, for a given n, the maximum allowed size of a cycle is upper bounded by 3n.

3 Contextuality with Pauli cycles

Clearly, no cycle realized by Pauli operators can exhibit strong contextuality since the operators over it are independent. This opens door to consider weaker arguments where we derive NC inequalities and check for the existence of quantum states that lead to the violation of atleast one of these inequalities.

Luckily, commutation properties in section 1.1 and 1.2 above turn out to be enough to characterise contextuality witnessing. The first step in every proof below takes inspiration from Tsirelson's original idea of squaring the operator to derive quantum bound for the CHSH inequality. We dedicate these proofs to his contribution to the field of quantum foundations.

For $k \geq 4$, all k-cycle NC inequalities were characterised by Araújo et.al. in [3]:

$$\Omega = \sum_{i=0}^{k-1} \gamma_i \langle A_i A_{i\oplus 1} \rangle \overset{NCHV}{\leq} k-2$$

where $\{A_i | i = 0, 1, ..., k-1\}$ is a set of measurements such that $[A_i, A_{i\oplus 1}] = 0$ and $\gamma_i \in \{\pm 1\}$ with odd number of $\gamma_i's$ always taking value -1. We start with a few instantiations of particular cycles before presenting a general proof later on.

3.1 The 4-cycle case

We start off by constructing the Bell-like operators corresponding to the inequalities of the 4-cycle, with the NC bound 2:

$$\Omega = \sum_{i=0}^{3} \gamma_i \langle A_i A_{i\oplus 1} \rangle \overset{NCHV}{\leq} 2$$

For the n,4-cycle, the relevant quantum operator appears as follows:

$$\langle Z \rangle = \gamma_0 \langle P_0 P_1 \rangle + \gamma_1 \langle P_1 P_2 \rangle + \gamma_2 \langle P_2 P_3 \rangle + \gamma_3 \langle P_3 P_4 \rangle$$

Since, we introduced the edge Paulis already above, the operator Z can be written in terms of them as follows:

$$Z = \gamma_0 L_0 + \gamma_1 L_1 + \gamma_2 L_2 + \gamma_3 L_3$$

The condition for contextuality of the Paulis then becomes:

$$\langle Z \rangle > 2$$

So, if we can find some that $|\Psi\rangle$ that gives the expectation value above 2 means those statistics don't have a non-contextual hidden variable explanation. We square the operator obtained above:

$$Z^2 = (\gamma_0 L_0 + \gamma_1 L_1 + \gamma_2 L_2 + \gamma_3 L_3)^2$$

For brevity, we write Z as:

$$Z = a + b$$

where $a = \gamma_0 L_0 + \gamma_1 L_1, b = \gamma_2 L_2 + \gamma_3 L_3$.

Therefore $Z^2 = (a+b)^2 = a^2 + b^2 + ab + ba$. Here,

$$a^2 = \gamma_0^2 L_0^2 + \gamma_1^2 L_1^2 + \gamma_0\gamma_1\{L_0, L_1\}$$

$$b^2 = \gamma_2^2 L_2^2 + \gamma_3^2 L_3^2 + \gamma_2\gamma_3\{L_2, L_3\}$$

$$ab + ba = \gamma_0\gamma_2\{L_0, L_2\} + \gamma_0\gamma_3\{L_0, L_3\} + \gamma_1\gamma_2\{L_1, L_2\} + \gamma_1\gamma_3\{L_1, L_3\}$$

Using ${\gamma_i}^2 = 1$ and further the edge Pauli commutation(anti) relations derived in section 4.1: $\{L_0, L_1\} = \{L_0, L_3\} = 0 = \{L_2, L_3\} = \{L_2, L_1\}$ and $[L_0, L_2] = 0 = [L_1, L_3]$, implies:

$$a^2 = 2I$$

$$b^2 = 2I$$

$$ab + ba = \gamma_0\gamma_2\{L_0, L_2\} + \gamma_1\gamma_3\{L_1, L_3\} = 2\gamma_0\gamma_2(L_0 L_2) + 2\gamma_1\gamma_3(L_1 L_3)$$

$$Z^2 = 4I + 2\gamma_0\gamma_2 L_0 L_2 + 2\gamma_1\gamma_3 L_1 L_3$$

We can further simplify this expression by noting that the commutation relations of the 4-cycle Paulis follow:

$$L_1 L_3 = P_1 P_2 P_3 P_0 = -P_0 P_1 P_2 P_3 = -L_0 L_2$$

This simplifies Z^2 as follows:

$$Z^2 = 4I + 2L_1 L_3(\gamma_0\gamma_2 - \gamma_1\gamma_3)$$

We know that there are only odd number of is s.t. $\gamma_i = -1$, hence for a 4-cycle two cases exist: (i) only one i s.t. $\gamma_i = -1$ (ii) three is s.t.$\gamma_i = -1$.
If (i) is true, then:

$$Z^2 = 4I + 4L_1 L_3 = 4(I + L_1 L_3) \qquad \text{(where } \gamma_1 \text{ or } \gamma_3 \text{ is -1)}$$

$$Z^2 = 4I - 4L_1 L_3 = 4(I - L_1 L_3) \qquad \text{(where } \gamma_0 \text{ or } \gamma_2 \text{ is -1)}$$

If (ii) is true, then:

$$Z^2 = 4I + 4L_1 L_3 = 4(I + L_1 L_3) \qquad \text{(where } \gamma_1 \text{ or } \gamma_3 \text{ is 1)}$$

$$Z^2 = 4I - 4L_1 L_3 = 4(I - L_1 L_3) \qquad \text{(where } \gamma_0 \text{ or } \gamma_2 \text{ is -1)}$$

We get the same conditions from both the possibilities. Also, note that $L_1 L_3$ produces some Pauli operator in $\mathcal{P}_n$. Therefore, for every case the maximum eigenvalue of Z^2 is 8. Therefore maximum eigenvalue of Z is $\sqrt{8}$ i.e. $+2\sqrt{2}$ or $-2\sqrt{2}$. When $Z = -2\sqrt{2}$, for a given inequality, then $Z = 2\sqrt{2}$ for a valid inequality which is a negative multiple of the initial one. Moreover, the state corresponding to this maximal violation is an eigenstate of the Pauli $L_1 L_3 = -P_0 P_1 P_2 P_3$. This means that for every 4-cycle, each Pauli realization maximally violates all the 4-cycle NC inequalities for some state for each inequality.

3.2 The 5-cycle case

In the 5-cycle case the quantum operator (Z) appears as follows:

$$Z = \gamma_0 L_0 + \gamma_1 L_1 + \gamma_2 L_2 + \gamma_3 L_3 + \gamma_4 L_4$$

Squaring the operator, gives:

$$Z^2 = 5I + \sum \gamma_i\gamma_k\{L_i, L_k\}$$

where the summation on r.h.s is over all combinations (i,k) s.t. $i \neq k$. We know from section 1.2 that for $k = 5$, all pair of distinct edge Paulis anti-commute, hence:

$$Z^2 = 5I$$

This means that the maximum eigenvalue of Z is $\sqrt{5} < 3$. This holds for all inequalities. Therefore the n,5-cycle never produces a contextual behaviour for any n.

3.3 The general case of k-cycles with $k > 4$

From the specific examples above we can notice that once we square the operator Z the only terms that survive among the anti-commutators are the ones where the edge Paulis commute with each other. For any $k \geq 5$ cycle:

$$Z = \sum_{i=0}^{k-1} \gamma_i L_i$$

The condition for contextuality becomes $\langle Z \rangle_{|\Psi\rangle} > k - 2$.

$$Z^2 = kI + \sum \gamma_i \gamma_k \{L_i, L_k\}$$

where the summation hold for all combinations (i,k) s.t. $i \neq k$. As noted in the 5-cycle case, within the summation on the r.h.s the anti-commuting pairs don't contribute but each commuting term appears as $2\gamma_i \gamma_k L_i L_k$.

$$Z^2 = kI + \sum 2\gamma_i \gamma_k L_i L_k$$

Now, we only need the count of such surviving terms to present our proof. We count as follows (use figure 2 to visualize the arguments below). Note that each L_i commutes with $k - 5$ other edge Paulis (excluding itself) in the cycle. We need to count the unique number of such pairs:

1. L_0, L_1, L_2 each commutes with $k - 5$ other edge paulis .
2. For L_3 we need to avoid redundancy and discount any commutation with Paulis in 1. We have $(k - 5) - 1 = k - 6$ commutations i.e. we excluded one with L_0.
3. For L_4 we need to exclude the commutation with L_0 & L_1. Hence $(k-5)-2 = k-7$ such relations.
4. We keep going like this, we reach L_{k-4} where only 1 commutation relation needs to be counted i.e. with L_{k-1}.
5. Beyond that every edge Pauli commutation combination has already been counted for in the steps above.

This means that the total unique counts that contribute in the r.h.s (summation part) of Z^2 above are:

$$3(k - 5) + (k - 6) + (k - 7) + (k - 6) + ... + 1 = 2(k - 5) + \frac{(k - 5)(k - 4)}{2}$$

Clearly, this sum only makes sense for $k \geq 5$. Now, we try to derive an upper bound on the maximum eigenvalue of Z^2 operator defined above:

$$\langle Z^2 \rangle_{|\Psi\rangle} = k + \sum 2\gamma_i \gamma_k \langle L_i L_k \rangle_{|\Psi\rangle}$$

If we try to compute the algebraic upperbound of r.h.s above by noting that each term in the summation is ≤ 1 (can't all together be 1 since all the Paulis across terms don't pairwise commute), Therefore:

$$\langle Z^2 \rangle_{|\Psi\rangle} < k + 2\{2(k - 5) + \frac{(k - 5)(k - 4)}{2}\} = k^2 - 4k$$

Therefore,

$$0 \leq \text{eig.val.}(Z^2) < k^2 - 4k$$

where eig.val.$(Z^2) \equiv$ any eigenvalue of operator Z^2. This also means that:

$$-\sqrt{k^2 - 4k} < \text{eig.val.}(Z) < \sqrt{k^2 - 4k}$$

For non-contextuality it must be that for all states $|\Psi\rangle$ in $\mathcal{H}_2^{\otimes n}$:

$$\langle Z \rangle_{|\Psi\rangle} \leq (k - 2)$$

Hence, condition for non-contextuality means that:

$$\sqrt{k^2 - 4k} < k - 2$$

which always holds true. Hence $\langle Z \rangle_{|\Psi\rangle} < k-2$ ($\forall$ $k \geq 5$ and $|\Psi\rangle$). This means that the statistics obtained from any Pauli k-cycle with $k \geq 5$ always lies strictly inside the classical (NC) polytope ($\forall$ $k \geq 5$).

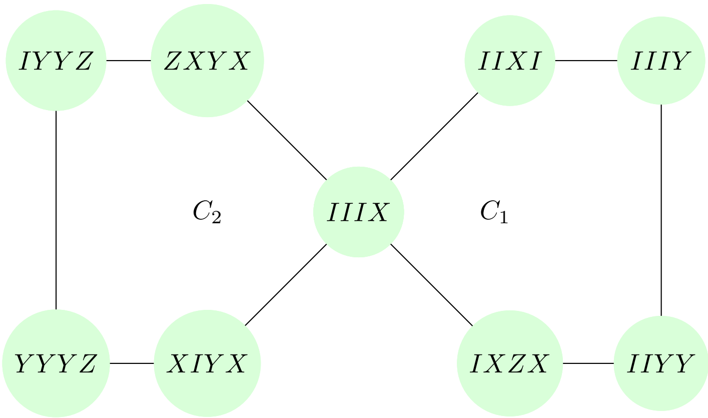

Figure 4: Two 5-cycles joined together at a node : a graph achievable only with $n \geq 4$. No such arrangement of Paulis can ever produce contextuality.

4 General compatibility graphs

4.1 Implication of 4-cycle contextuality on a general scenario

The proofs above imply that if a graph has atleast one 4-cycle as its induced subgraph, then there always exists a quantum state that produces statistics indescribable by any non contextual model. We can prove this by the following argument: Imagine that $G_{\mathcal{M}}$ is a graph with an induced 4-cycle and assume that it produces only non-contextual statistics. This means that a JPD over $\mathcal{M}$ exists that explains all the statistics one can observe over any subgraph by marginalization (over the rest of the graph). If we now take some state $|\Psi\rangle$ such that it violates one of the 4-cycle NC inequalities in the graph, we can arrive at a contradiction with our assumption. By the assumption of non-contextuality of the whole graph there always ($\forall \ |\Psi\rangle \in \mathcal{H}_2^{\otimes n}$) exists a JPD over every 4-cycle (obtained by marginalisation). But we know that this is impossible since violation of NC inequalities for 4-cycles implies impossibility of a JPD over a 4-cycle. Hence, the assumption is contradicted and $G_{\mathcal{M}}$ can produce contextuality[6].

This raises a natural question: Given an arbitrary Pauli compatibility graph with atleast one induced k-cycle ($k \geq 5$), can it produce contextuality? For graphs where there is exactly one such cycle, it's not complicated to construct a JPD but for generic graphs, one has to be careful. Answer to the above question relates with the answer to another important question: What is the precise role of induced cycles within compatibility graphs in producing contextuality? As discussed in section 4, we know that presence of cycles ensures that one can always find some quantum observables such that the whole graph produces atleast as much contextuality as the cycle. We know that the Pauli cycles in question alone don't produce contextuality but despite that the overall Pauli graph may still be able to exhibit contextuality. We explore this using graphs that can be seen as different combinations of two 5-cycles.

4.2 Combo of two 5-cycles

We consider three cases where two 5-cycles conjoin together differently.

Case I: Only one node is common as depicted in figure 3.
Clearly, such a Pauli-graph always has a non-contextual model. This is because a JPD over it (P_T) exists:

$$P_T = \frac{P_{C_1} P_{C_2}}{P_A}$$

where P_{C_i} is a JPD for i^{th} cycle and P_A is probability for outcomes of A alone. Due to no-disturbance the common node A has a unique probability distribution.

[6]More than anything, this proof underlines that adding more Paulis in addition to the 4-cycle in no way nullifies (or decreases) the contextuality witnessing effects of the 4-cycle.

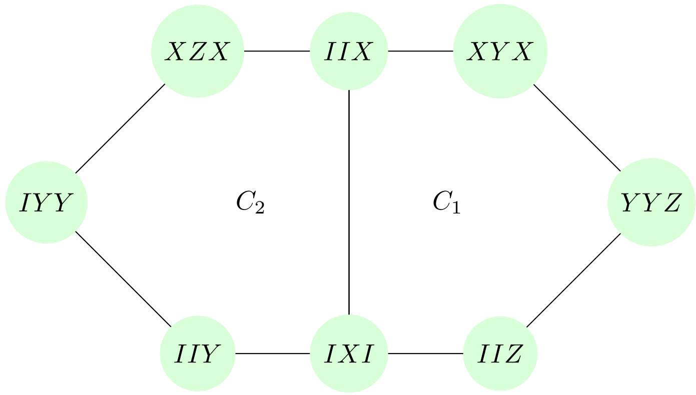

Figure 5: Two 5-cycles joined together : a graph achievable only for $n \geq 3$. Such a graph of Paulis can't produce contextuality for any such arrangement of Paulis.

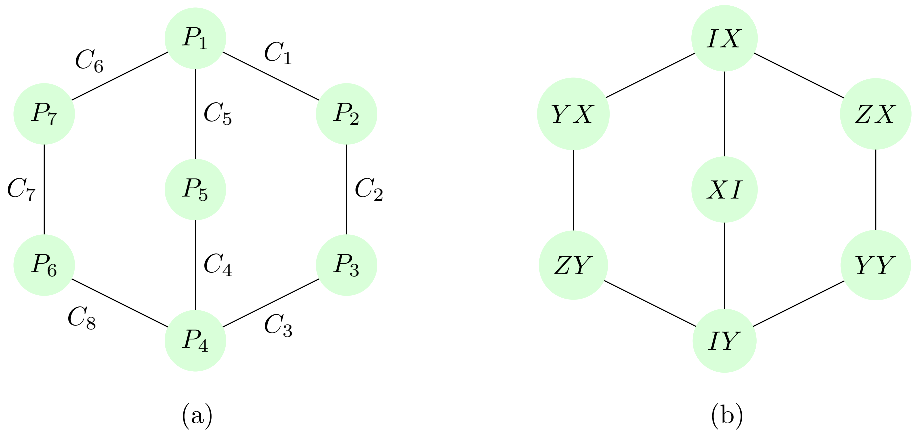

Figure 6: Two 5-cycles sharing two edges (C_5, C_4): a graph achievable $\forall\, n \geq 2$: (a) represents the generic n-qubit Paulis and respective contexts (C_i). (b) exemplifies one such cycle with Paulis that violate the NC inequality. Notice that unlike previous figures where C represented cycle, here in (a) C_i represents i^{th} context.

Case II: Two cycles share an edge as depicted in figure 4.
This Pauli-graph always possesses a non-contextual model due to the existence of a JPD(P_T) over it:

$$P_T = \frac{P_{C_1} P_{C_2}}{P_{AB}}$$

where P_{C_i} is a JPD for i^{th} cycle and P_{AB} is JPD over the common context AB. Due to no-disturbance the common context AB has a unique probability distribution.

Case III: The two 5-cycles conjoin together with two edges in common. This case becomes non-trivial because now there is no guarantee that the JPDs over the two cycles give the same marginals for the unmeasurable correlation (AC). Due to no-signalling the JPDs over the two cycles are constrained to give the same overlap for the common contexts AB and BC. But since AC is not a context the same doesn't hold for it. To check for this we used, PORTA software package [5] to obtain all the NC inequalities corresponding to this graph. Using the Paulis illustrated in figure 5(b), we observed a violation of one of the NC inequalities.

The following is the considered NC inequality:

$$\begin{aligned} &- P^{C_1}_{--} + P^{C_2}_{-+} + P^{C_3}_{-+} - P^{C_4}_{--} + (P^{C_5}_{-+} + P^{C_5}_{+-} + 2P^{C_5}_{--}) - \\ &\qquad P^{C_6}_{--} + (P^{C_7}_{-+} + P^{C_7}_{+-} + 2P^{C_7}_{--}) + (P^{C_8}_{+-} - P^{C_8}_{-+} + P^{C_8}_{--}) \leq 3 \end{aligned} \quad (1)$$

Here $P_{ab}^{C_i}$ represents probability of joint outcome ab on measuring the i^{th} context i.e. C_i. By translating the projectors of contexts to Pauli operators, we can translate this inequality into operator inequality, as follows:

$$-(P_1P_2 + P_2P_3 + P_3P_4 + P_4P_5 + P_1P_7) + P_4P_6 - (P_4 + P_5 + P_6 + P_7) \leq 4I$$

Using the Paulis in figure 5(b), the l.h.s above becomes:

$$-(ZI + XZ + YI + XY + YI) + ZI - (IY + XI + ZY + YX)$$

Now, if we check for the maximum eigenvalue of this expression, it turns out to be $4.2716 > 4$. Hence, a violation of the inequality. The corresponding state is: $(0.2787 - 0.5952i, -0.2787 - 0.3342i, -0.4092 + 0.1482i, -0.4352 + 0.0000i)^T$ in the computational basis. This implies that P_{AC} obtained from two cycles, after marginalisation, won't be unique.

Therefore, these conjoined cycles produce contextuality. This illustrates that the quantum violation of the NC inequalities for a given scenario (compatibility graph) doesn't necessarily accompany the violation of some induced cycle NC inequality within the graph. Hence, it seems that the fundamental role of an induced cycle in a compatibility graph of a fixed set of quantum measurements is only to preclude application of Vorob'ev's theorem to the graph. The chosen set of quantum measurements then may or may not produce contextuality.

There seems to be a better way to understand this in terms of the geometrical approach to NC correlations i.e. the correlation polytopes. In [12] the author showed that a facet-defining inequality for a Bell scenario(n, m, v)[7] remains a facet-defining inequality for any Bell scenario(n', m', v') where $n' \geq n, m' \geq m, v \geq v'$. Assuming that this idea of preservation of facet, as the scenario becomes a sub-scenario of a bigger scenario, generalises to NC correlations too. Then, one can say that the cycle-inequalities are just a proper subset of all inequalities for the whole scenario in case III. The contextuality observed with Pauli operators, in case III, is then just the violation of an inequality outside this proper subset. In this light, the role of induced cycles in an arbitrary graph doesn't seem so mysterious.

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[7] n= no. of parties, m= no. of measurements per party, v = no. of outcomes of measurements

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