## 1 Pauli operators on cycles

To answer what k-cycles are Pauli realizable, for a given n, we developed on our guiding intuition that introducing edge Pauli operators over a 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 other details, we start with some notational clarification:  $\mathcal{P}_{\mathbf{n}}$  will denote  $\pm 1$  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.

#### 1.1 Forbidden Edge Paulis

- No Edge Pauli can be the same as any of the cycle Paulis constituting it:  $L_i = P_i P_{i \oplus 1}$  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.  $L_i = P_i P_{i \oplus 1} \neq \pm P_l$  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 at least 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.

#### 1.2 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<sup>1</sup> 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  $i \oplus 3 \le j \le i \oplus (k-3)$  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  $i \oplus 2$ .

#### 1.3 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.

<sup>&</sup>lt;sup>1</sup>nearest w.r.t indices

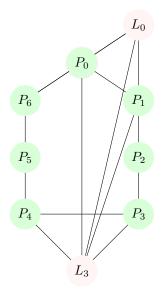


Figure 1: In the 2,7-cycle of Paulis (in green) we introduce two edge Paulis (in pink)  $L_0 = P_0 P_1$ ;  $L_3 = P_3 P_4$  and some more edges allowed by the four conditions obtained in section 4.1.

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.
- $\alpha = 1, \beta = 0 \implies L_3 = P_0$ : 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.
- $\alpha = 1, \beta = 1 \implies L_3 = P_0L_0 = P_0P_0P_1 = P_1$ : 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 at least 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<sup>2</sup>: 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.  $S_i \equiv \{P_0, L_0, L_3, L_6, ... L_{i-3}, L_i\}$ .

<sup>&</sup>lt;sup>2</sup>independent means that no Pauli operator can be written as a product of other commuting Paulis

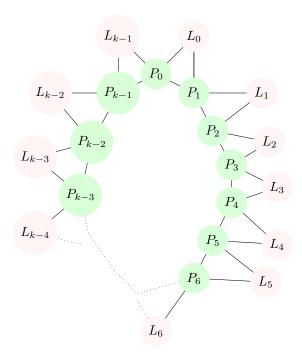


Figure 2: An arbitrary n,k-cycle (green) and edge Paulis  $L_i = P_i P_{i \oplus 1}$  (pink), the dotted lines refers to the Paulis (including edge Paulis) not drawn but are part of the cycle.

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  $P_0, L_0$  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  $|S| \le n$ . 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.

# 2 Contextuality of n,k 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 [?]:

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

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.

#### 2.1The n,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:

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

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:  $\{L_0, L_1\} = 1$  $\{L_0, L_3\} = 0 = \{L_2, L_3\} = \{L_2, L_1\}$  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:

$$L_1L_3 = P_1P_2P_3P_0 = -P_0P_1P_2P_3 = -L_0L_2$$

This simplifies  $Z^2$  as follows:

$$Z^2 = 4I + 2L_1L_3(\gamma_0\gamma_2 - \gamma_1\gamma_3)$$

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:

$$Z^2 = 4I + 4L_1L_3 = 4(I + L_1L_3)$$
 (where  $\gamma_1$  or  $\gamma_3$  is -1)

$$Z^2 = 4I - 4L_1L_3 = 4(I - L_1L_3)$$
 (where  $\gamma_0$  or  $\gamma_2$  is -1)

If (ii) is true, then:

$$Z^2 = 4I + 4L_1L_3 = 4(I + L_1L_3)$$
 (where  $\gamma_1$  or  $\gamma_3$  is 1)

$$Z^2 = 4I - 4L_1L_3 = 4(I - L_1L_3)$$
 (where  $\gamma_0$  or  $\gamma_2$  is -1)

We get the same conditions from both the possibilities. Also, note that  $L_1L_3$  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  $L_1L_3=-P_0P_1P_2P_3$ . This means that for every 4-cycle, each Pauli realization maximally violates all the 4-cycle NC inequalities for some state for each inequality.

### 2.2 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.

## 2.3 The general case for the k-cycle $\forall k \geq 5$

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  $2\gamma_i\gamma_kL_iL_k$ .

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

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:

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

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  $\leq 1$  (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,

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

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

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

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

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

Hence, condition for non-contextuality means that:

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

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

# 3 General Compatibility graphs

#### 3.1 Implication of 4-cycle contextuality on a general scenario

The proofs above imply that if a graph has at least 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<sup>3</sup>.

This raises a natural question: Given an arbitrary Pauli compatibility graph with at least 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 at least 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.

<sup>&</sup>lt;sup>3</sup>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.

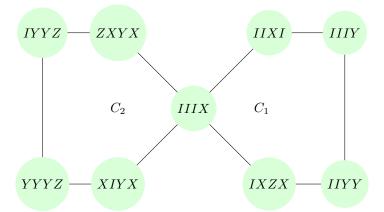


Figure 3: Two 5-cycles joined together at a node : a graph achievable only with  $n \geq 4$ . No such arrangement of Paulis can ever produce contextuality.

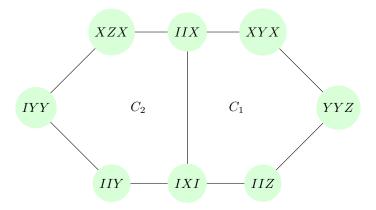


Figure 4: Two 5-cycles joined together : a graph achievable only for  $n \ge 3$ . Such a graph of Paulis can't produce contextuality for any such arrangement of Paulis.

#### 3.2 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.

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

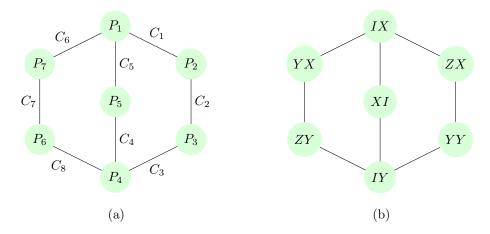


Figure 5: Two 5-cycles sharing two edges  $(C_5, C_4)$ : a graph achievable  $\forall n \geq 2$ : (a) represents the generic n-qubit Paulis and respective contexts  $(C_i)$ . (b) exemplifies one such cycle with Paulis that violate the NC inequality. Notice that unlike previous figures where C represented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

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 [?] 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:

$$\begin{split} -P_{--}^{C_1} + P_{-+}^{C_2} + P_{-+}^{C_3} - P_{--}^{C_4} + (P_{-+}^{C_5} + P_{+-}^{C_5} + 2P_{--}^{C_5}) - \\ P_{--}^{C_6} + (P_{-+}^{C_7} + P_{+-}^{C_7} + 2P_{--}^{C_7}) + (P_{+-}^{C_8} - P_{-+}^{C_8} + P_{--}^{C_8}) \leq 3 \end{split} \tag{1}$$

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:

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

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 together 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 [?] the author showed that a facet-defining inequality for a Bell scenario $(n, m, v)^4$  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.

 $<sup>^4</sup>$ n= no. of parties, m= no. of measurements per party, v = no. of outcomes of measurements