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## Supplemental Materials

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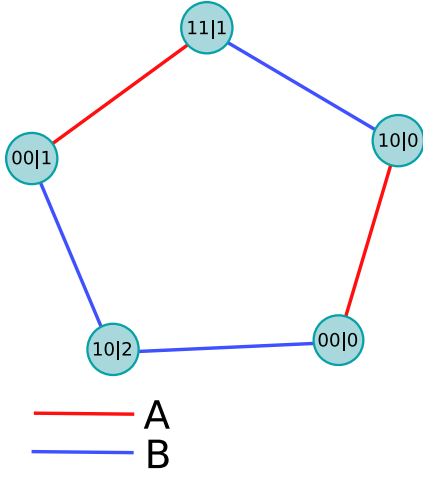


Figure 1: Edge colored exclusivity graph representation of the Bonet inequality. Exclusivity constraints for the party  $A$  and  $B$  are represented by red lines and blue lines respectively.

### Building the exclusivity graph from DAG

In the following we describe in more details how to get from the DAG (Directed Acyclic Graph) representation of a causal model to the one for exclusivity graph. Starting from a generic causal model described by a DAG  $D$ , with  $N$  random variables  $O_D = \{A_1, \dots, A_N\}$  and  $M$  instruments  $I_D = \{X_1, \dots, X_M\}$ , the exclusivity graph  $G = (V, E)$  can be constructed, for example, using a simple breadth-first graph exploring algorithm. The procedure, described in algorithm 1, requires the DAG  $D$  and the list  $V$  of vertices to be explored, since we can be interested in building the graph only for a subset of events.

### Edge colored multigraph technique for approximating the quantum bound

The Lovász theta of a graph, despite being efficiently computable, only gives an upper bound to the maximal quantum bound, since it ignores the additional constraints arising from the presence of different random variables  $A_i$ . Indeed the quantum bound is influenced not only by the exclusivity relations between the possible events in our scenario, but also on how those relations are derived from the variables  $A_1, \dots, A_N$ .

To obtain a better approximation for the quantum bound we can follow the technique presented in [1]. This method consists in introducing an edge coloring in the exclusivity graph. This edge coloring encodes the information of which of the  $A_i$ s is involved in the exclusivity constraints under consideration. In practice this corresponds to constructing an exclusivity graph  $G_i$  for each  $A_i$ . The resulting object is called a *multigraph*. Having defined a multigraph  $G = G_1, \dots, G_N$  for a given scenario the quantum bound is defined by the quantity:

$$\vartheta(G) = \max_v \sum_{i \in V} |v \cdot a_i^1 \otimes \dots \otimes a_i^n|^2 \quad (1)$$

where  $\{a_i^j\}$  is an orthonormal labelling for  $G_j$  and  $V$  is the set of vertices of  $G$ . This quantity, which can be seen as a generalization of the Lovász theta, is in general not efficiently computable, but, as described in [1], can be arbitrarily approximated by a hierarchy of semi-definite programs[2].

For example, in the case of the pentagon in the instrumental scenario we have two colors, and thus two graph  $G_A$  and  $G_B$ , corresponding to variables  $A$  and  $B$  respectively, as shown in Fig. 1. Applying the technique described above to this scenario yields a quantum bound of 2.2071, reproducing the known value for the quantum bound of the Bonet inequality given by  $(3 + \sqrt{2})/2$ .

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**Algorithm 1** Breadth-first graph exploration

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1: function BUILD GRAPH( $V, D$ )
2:    $E \leftarrow \emptyset$ 
3:   while  $V \neq \emptyset$  do
4:     INSERT( $Q, V_1$ ) ▷ Initialize the queue with the first element of  $V$ 
5:     DELETE( $V, V_1$ )
6:     while  $Q \neq \emptyset$  do
7:        $v \leftarrow Q_1$ 
8:       DELETE( $Q, Q_1$ )
9:       for  $u \in V$  do
10:        if EXCLUSIVE( $u, v$ ) then
11:          INSERT( $E, (v, u)$ )
12:          INSERT( $Q, u$ )
13:          DELETE( $V, u$ ) ▷ Visited nodes are removed from  $V$ 
14:        end if
15:      end for
16:    end while
17:  end while
18:  return  $E$ 
19: end function
```

As in the main text, here  $a, a'$  stand for the value of the outcome of the variable  $A$  in the events  $v, v'$ , while  $p_a, p_{a'}$  stand for the values of the parent nodes of  $A$  in  $D$ ,  $\text{PA}(A)$ .

```
1: function EXCLUSIVE( $v, v', D$ )
2:    $n \leftarrow \text{true}$ 
3:   for  $A \in O_D$  do
4:      $n \leftarrow n \wedge (p_a \neq p_{a'} \vee (p_a = p_{a'} \wedge a = a'))$ 
5:   end for
6:   return  $\neg n$ 
7: end function
```

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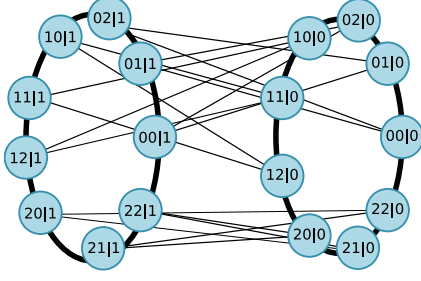


Figure 2: Exclusivity graph for the instrumental scenario 233, showing the impossibility of having cycles with more than 5 vertices. To simplify the figure cliques are represented by bold lines between vertices.

### There are no quantum violation for instrumental scenarios with $l = 2$ settings.

It is easy to see that no quantum violation is possible for instrumental scenario with  $l = 2$  possible settings for the instrumental variable  $X$ . This reduces to proving that there are no odd  $n$ -cycles nor  $n$ -anticycles as induced subgraphs in the corresponding exclusivity graph, with  $n \geq 5$ . To see this we can notice that any such graph is composed by two cliques (see for example Fig. 2), corresponding to the events with  $x = 0$  and  $x = 1$ . Any  $n$ -cycle with at least 5 vertices must then have at least 3 mutually connected vertices belonging to the same  $x$ , so they can never form a cycle-graph. Similarly we can show that there cannot be any induced odd anticycle with 5 or more vertices.

### There are no cycles $C_n$ with $n \geq 7$ in the $l22$ instrumental scenario.

In the following we prove that there cannot be a odd anticycle with more than 5 vertices in the exclusivity graph associated to an instrumental scenario of the type  $l22$ .

Two different events  $ab|x$  and  $a'b'|x'$ , are exclusive if one of these two conditions is true:

1.  $x = x'$ .
2.  $a = a'$  and  $b \neq b'$ .

Suppose we have a cycle  $C_n$  with  $n \geq 7$ , as in fig. 3, and consider that node 2 in this graph corresponds to an event which we can arbitrarily identify as  $00|0$ . Among its neighbors 1 and 3, one will necessarily need to satisfy rule 2 (they cannot both satisfy rule 1 or the three nodes would be a clique). So without loss of generality we can assign the event  $01|1$  to 3. Since nodes 5, 6, 7 must not satisfy rule 2 with both 2 and 3, then they must have

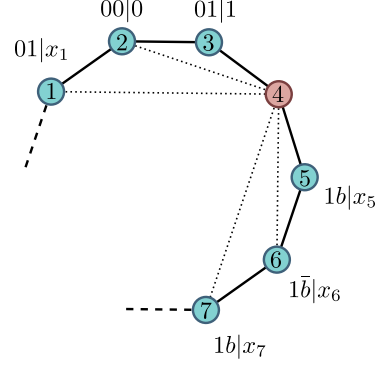


Figure 3: Proof of the impossibility of having cycles with 7 nodes or more in the  $d22$  scenario.

$a = 1$ . Moreover 7 and 5 must have the same  $b$ , different from 6. In the same way 1 must not satisfy rule 2 with 6, 5 and 3, so it needs to have  $a = 0$  and  $b = 1$ . At this point, since we only have values  $\{0, 1\}$  for  $a$ , we cannot avoid node 4 to be linked to one of the nodes 1, 2, 6, 7. Thus, the corresponding graph cannot be a cycle.

### References

- [1] R. Rabelo, C. Duarte, A. J. López-Tarrida, M. T. Cunha, A. Cabello, *Multigraph approach to quantum non-locality*. Journal of Physics A: Mathematical and Theoretical, 47, 424021 (2014).
- [2] M. Navascués, S. Pironio, & A Acín, *A convergent hierarchy of semidefinite programs characterizing the set of quantum correlations*. New Journal of Physics 10, 073013 (2008).