Quantum Foundations for a Large Class of Graphs

Thiago Assis e Gabriel Coutinho

***Abstract*— In the graph-theoretic approach to contextuality, a key problem is to give a foundational justification for quantum theory from some simple physical principles. This was already solved for perfect graphs. We investigate whether assuming this to hold for minimally imperfect graphs implies it for all imperfect graphs. We confirm this hypothesis for a large family of graphs, $\mathcal{G}$, which contains all minimally imperfect graphs and is closed under complement, disjoint union, and addition of twins. Our proof relies on a new characterization of the theta body of a graph under the addition of twins.**

***Keywords*— contextuality, quantum correlations, graph theory, exclusivity principle**

I. Introduction

Two events are said to be exclusive if they cannot occur simultaneously, meaning there exists a measurement for which the events yield different outcomes. Based on this, we can construct a graph G, called the graph of exclusivity. The vertex set of G represents the set of events, and an edge connects two vertices if and only if the corresponding events are exclusive (see [5] for a complete reference on the topic).

What are the possible results of an experiment? From a fixed initial state, we can obtain a vector $\mathbf{p} \in \mathbb{R}^{V(G)}$, called a behavior for G, where $\mathbf{p}_v$ is the probability of event $v \in V(G)$ occurring, given the fixed initial state. The set of all possible behaviors depends on the adopted physical theory.

A. Cabello showed [1] that the set of behaviors defined by classical theory, quantum theory, and the E-Principle (to be explained further) are, respectively, the following convex bodies, well known in the theory of polyhedral optimization and semidefinite programming.

$$\text{STAB}(G) = \text{ConvHull}\Big\{\mathbf{1}_S : \ S \subseteq V(G), S \text{ independent}\Big\}. \tag{1}$$

$$\begin{aligned}\text{TH}(G) = \Big\{\mathbf{x} : \begin{pmatrix} 1 & \mathbf{x} \\ \mathbf{x}^T & X \end{pmatrix} \succcurlyeq 0,\\ X_{vu} = 0 \ \forall \ vu \in E(G),\\ X_{vv} = \mathbf{x}_v \ \forall \ v \in V(G)\Big\}.\end{aligned} \tag{2}$$

$$\text{QSTAB}(G) = \left\{\mathbf{y} : \mathbf{1}_C^T \mathbf{y} \le 1 \text{ for every clique } C\right\}. \tag{3}$$

These sets satisfy the following relation:

$$\text{STAB}(G) \subseteq \text{TH}(G) \subseteq \text{QSTAB}(G). \tag{4}$$

The E-Principle (EP) states that if $S \subseteq V(G)$ is a set of mutually exclusive events, then $\mathbf{1}_S^T p \le 1$ for any behavior.

We now introduce our main object. If G is a graph representing exclusive events, we define $X(G) \subseteq \mathbb{R}^{V(G)}$ to be the set of behaviors allowed in our reality. Assuming the EP, when applied to a single graph, it gives $X(G) \subseteq \text{QSTAB}(G)$.

However, it is reasonable to extend this principle to scenarios where experiments are being performed simultaneously. Given the graphs of exclusivity G, H for two experiments conducted independently, we define the OR product as the graph $G * H$ with vertex set $V(G) \times V(H)$, and edges $(g_1, h_1) \sim (g_2, h_2)$ exactly when $g_1 \sim_G g_2$ or $h_1 \sim_H h_2$. Moreover, if $\mathbf{p} \in X(G)$ and $\mathbf{q} \in X(H)$, then $\mathbf{p} \otimes \mathbf{q} \in X(G * H)$. With this, the EP can be reinstated in its stronger version as:

$$\text{ConvHull}\left[X(G) \times X(H)\right] \subseteq \text{QSTAB}(G * H). \tag{5}$$

This formulation provides a powerful constraint on physical theories satisfying the EP. A result from Amaral et al. [5] uses this to show:

Theorem 1: Let G be a graph such that $\text{TH}(\overline{G}) \subseteq X(\overline{G})$. The EP implies that $X(G) \subseteq \text{TH}(G)$.

Note that if we assume quantum theory as a principle, i.e., $\text{TH}(G) \subseteq X(G)$ for all graphs G, then Theorem 1 implies $\text{TH}(G) = X(G)$. However, assuming quantum theory is arguably too strong as a premise [2]. We explore whether we can justify $X(G) = \text{TH}(G)$ under weaker assumptions.

II. Results

Besides the EP, the following principles are also intuitive, and heavily used in the literature:

$$X(G) \text{ is isomorphism invariant.} \tag{6}$$

$$X(G) \text{ is a convex corner.} \tag{7}$$

$$\text{STAB}(G) \subseteq X(G). \tag{8}$$

A convex corner is a compact and convex set $S \subseteq \mathbb{R}^n_+$ that is also down monotone, i.e., if $\mathbf{w} \in S$ and $0 \le \mathbf{z} \le \mathbf{w}$, then $\mathbf{z} \in S$.

V. Chvátal's characterization of perfect graphs [4], allied with principles (5) and (8), is able to justify $X(G) = \text{TH}(G)$ for all perfect graphs. Thus, what remains to consider are the imperfect graphs. Taking $X(G) = \text{STAB}(G)$ satisfies all the principles mentioned. However, there are quantum mechanic experiments which exhibits behaviours $\mathbf{p}$ for imperfect graphs for which $\mathbf{p} \in \text{TH}(G) \setminus \text{STAB}(G)$, see [3].

The Perfect Graph Theorem [6] states that a graph is imperfect if and only if it has an odd cycle C_n or the complement of an odd cycle $\overline{C}_n$ as an induced subgraph for some $n \ge 5$. Thus, the odd cycles and their complements can be viewed as the building blocks of imperfect graphs. This motivates the following question: if we assume quantum behaviours for the minimally imperfect graphs, can we show

Thiago Assis, Dept. of Computer Science, Universidade Federal de Minas Gerais, Belo Horizonte-MG, e-mail: thiago.assis@dcc.ufmg.br; Gabriel Coutinho, Dept. of Computer Science, Universidade Federal de Minas Gerais, Belo Horizonte-MG, e-mail: gabriel@dcc.ufmg.br;

that $\text{TH}(G) = X(G)$ for all imperfect graphs? Therefore, from now on, we assume that

$$\text{TH}(G) \subseteq X(G) \text{ for any minimally imperfect graph } G \quad (9)$$

We are not able to answer this question in its full version. However, in this work we present a justification of $X(G) = \text{TH}(G)$ for a large class of imperfect graphs.

Let G be a graph and $v \in V(G)$. A false twin is a vertex v' that shares all its neighbors with v, but is not connect to v. A true twin also shares the neighborhood, but now v and v' are connected. Let G_v^f be the graph obtained from G by creating a false twin for v, and G_v^t bt the graph obtained from G by creating a true twin for v. The theta body of G_v^f and G_v^t can be characterized in terms of the theta body of G:

Theorem 2: The vector $(x_v, x_{v'}, \mathbf{x}) \in \text{TH}(G_v^f)$ if and only if $(\max(x_v, x_{v'}), \mathbf{x}) \in \text{TH}(G)$.
Proof: Without loss of generality, assume $x_v \geq x_{v'}$. As $G \subseteq G_v^f$, we have $(x_v, \mathbf{x}) = (\max(x_v, x_{v'}), \mathbf{x}) \in \text{TH}(G)$.

For the reverse implication, take $(\max(x_v, x_{v'}), \mathbf{x}) \in \text{TH}(G)$. Since $v \not\sim v'$, we can just copy the orthonormal representation of v to v', yielding $(\max(x_v, x_{v'}), \max(x_v, x_{v'}), \mathbf{x}) \in \text{TH}(G_v^f)$. Using the fact that the theta body is down monotome, we get $(x_v, x_{v'}, \mathbf{x}) \in \text{TH}(G_v^f)$. ■

Theorem 3: The vector $(x_v, x_{v'}, \mathbf{x}) \in \text{TH}(G_v^t)$ if and only if $(x_v + x_{v'}, \mathbf{x}) \in \text{TH}(G)$.
Proof: Let $(x_v + x_{v'}, \mathbf{x}) \in \text{TH}(G)$. As $G \subseteq G_v^t$, we may conclude that $(0, x_v + x_{v'}, \mathbf{x}) \in \text{TH}(G_v^t)$ and that $(x_v + x_{v'}, 0, \mathbf{x}) \in \text{TH}(G_v^t)$. Using the fact that the theta body is convex, we have $(x_v, x_{v'}, \mathbf{x}) \in \text{TH}(G_v^t)$.

For the forward implication, let $(x_v, x_{v'}, \mathbf{x}) \in \text{TH}(G)$. There must exist some matrix of the form

$$\begin{pmatrix} 1 & x_v & x_{v'} & \mathbf{x}^T \\ x_v & x_v & 0 & \mathbf{x}_v^T \\ x_{v'} & 0 & x_{v'} & \mathbf{x}_{v'}^T \\ \mathbf{x} & \mathbf{x}_v & \mathbf{x}_{v'} & X \end{pmatrix} \quad (10)$$

satisfying the restrictions for $\text{TH}(G_v^t)$ (defined in Equation 2). Adding the second and third rows and columns of the above gives:

$$\begin{pmatrix} 1 & x_v + x_{v'} & \mathbf{x}^T \\ x_v + x_{v'} & x_v + x_{v'} & \mathbf{x}_v^T + \mathbf{x}_{v'}^T \\ \mathbf{x} & \mathbf{x}_v + \mathbf{x}_{v'} & X \end{pmatrix}. \quad (11)$$

This matrix satisfies all restrictions for $\text{TH}(G)$, and so $(x_v + x_v', \mathbf{x}) \in \text{TH}(G)$. ■

This characterizations allows us to prove the following theorem, which is our main result:

Theorem 4: Let G' be a graph obtained from G by the addition of a twin for vertex $v \in V(G)$. If $\text{TH}(G) \subseteq X(G)$, then $\text{TH}(G') \subseteq X(G')$.
Proof: We will construct an experiment with G' as its graph of exclusivity. Then, we show that any behaviour $p \in \text{TH}(G')$ can be realized, and so $\text{TH}(G') \subseteq X(G)$. For this, we use the fact that $X(K_2) = \{(s,t) : s + t \leq 1\}$ and $X(\overline{K}_2) = \{(s,t) : s, t \leq 1\}$.

- If $G' = G_v^f$ (addition of a false twin), define the following experiment. Start by performing an experiment with graph of exclusivity G. If event v happens, then perform, in sequence, some experiment associated with $H = \overline{K}_2$. This new experiment has graph of exclusivity G'. Moreover, note that if $(p_v, \mathbf{p}) \in X(G)$, then $(p_v s, p_v t, \mathbf{p}) \in X(G')$ for any $s, t \leq 1$. Thus, by Theorem 2, we get $\text{TH}(G') \subseteq X(G')$.
- If $G' = G_v^t$ (addition of a true twin), we perform a simillar construction, but now with $H = K_2$. If $(p_v, \mathbf{p}) \in X(G)$, then $(p_v s, p_v t, \mathbf{p}) \in X(G')$ for any $s + t \leq 1$. Now apply Theorem 3, and this concludes the proof.

■

Let $\mathcal{G}$ be the graph family containing the odd cycles C_n with $n \geq 5$, and closed under complement, disjoint union, and creating twins. The assumption of $X(G) \subseteq \text{TH}(G)$ for all minimally imperfect graphs, together with Theorems 1 and 4 imply that $X(G) = \text{TH}(G)$ for all graphs $G \in \mathcal{G}$.

III. Conclusion

In this work, we searched for an intuitive physical principle that justifies $X(G) = \text{TH}(G)$. We investigated if this equality holding for minimally imperfect graphs would imply it holds for all imperfect graphs. While this general question remains open, we have shown that the implication is true for the graph family $\mathcal{G}$, the smallest class containing all minimally imperfect graphs that is closed under complement, disjoint union, and addition of twins. As a secondary result, we also provided a characterization for the theta body of a graph under the addition of twins.

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