Eur. Phys. J. D (2016) 70: 205
DOI: 10.1140/epjd/e2016-60577-y

THE EUROPEAN PHYSICAL JOURNAL D

Regular Article

Relations among non-chordal compatibility graphs, imperfect exclusivity graphs and quantum correlations*

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Received 13 October 2015 / Received in final form 31 August 2016
Published online 13 October 2016 –

Abstract. The relations among non-chordal compatibility graphs, imperfect exclusivity graphs and quantum correlations are investigated in the scenario where the compatibility relations and the events are fixed. In this scenario, we prove that the non-chordal compatibility graph is a sufficient condition for exhibiting quantum correlations and the imperfect exclusivity graph is an insufficient condition for exhibiting quantum correlations. The result provides a convenient tool to determine whether an observable set can distinguish the quantum from classical correlations.

Quantum contextuality is an important feature of quantum theory which is different from the non-contextual hidden variable (NCHV) theory [1–3]. This counterintuitive property can be indicated by the violations of non-contextuality inequalities [4–11]. It also can be demonstrated experimentally [12–17]. There is the difference between the quantum and the NCHV bound of a non-contextuality inequality since the observable set lacks the joint probability distribution [18,19].

Recently, the graph theory has been utilized in investigating the quantum correlations [20–29]. The exclusivity graph expresses the exclusivity relations among the measurement events of the non-contextuality inequalities [20–24]. Its vertices represent the events such as $(A_{k_1} = a_{k_1}, \dots, A_{k_s} = a_{k_s})$, where $\{A_{k_1}, \dots, A_{k_s}\}$ are jointly measurable. Two events can't happen simultaneously if they have the same observable A_i while its outcomes are different. Two vertices corresponding two exclusive events are adjacent in the exclusivity graph. The exclusivity graph can be utilized in bounding non-contextuality inequalities [20–26]. The imperfect exclusivity graph is the necessary and sufficient condition for exhibiting quantum correlations (which is not referred to any specific compatibility scenario) [23]. On the other hand, the compatibility relations among the observables of the non-contextuality inequalities can be expressed by the compatibility graph [27,28]. Each vertex represents an observable while the edge connecting two vertices indicates the two observables are compatible. The compatibility graph can also be applied in many investigations such as exhibitions of monogamy between non-contextuality inequalities [27], monogamy between non-contextuality inequality and locality inequality [28]. The observable set admits a joint probability distribution if the compatibility graph is a chordal graph [27]. In other words, the non-chordal graph is a necessary condition for singling out quantum correlations from classical correlations [18].

In this Letter, we investigate the relations among the non-chordal compatibility graph, the imperfect exclusivity graph and the necessary and sufficient condition for exhibiting quantum correlations in the scenario where the compatibility relation and the measurement events are fixed.

Compatibility-fixed(events-fixed) scenario: in the scenario we discussed here, when a non-contextuality inequality is fixed, the events indicated by the vertices of the exclusivity graph are fixed. Then the compatibility relations among the observables are fixed. Hence the compatibility graph is fixed if the events of the exclusivity graph are fixed. For example, an event $P(A_1 = 1, B_1 = -1)$ in the CHSH inequality [30,31] indicates the compatibility relation between the observable A_1 and the observable B_1. The compatibility among the observables in the CHSH inequality can be obtained as a square. On the other hand, the jointly measurable subsets are fixed if the compatibility among an observable set are fixed. Then, the events of this observable set are fixed. So the events of the exclusivity graph are fixed if the compatibility relations among the observables are fixed. We call this scenario the compatibility-fixed scenario or events-fixed scenario. Furthermore in this scenario, usually all observables only have outcomes +1 and −1. It is worthy noticing that the compatibility-fixed scenario (events-fixed) scenario is different from the scenario discussed in reference [23]. In this scenario, vertices of the exclusivity graph represent

* Supplementary material in the form of one pdf file available from the Journal web page at
http://dx.doi.org/10.1140/epjd/e2016-60577-y

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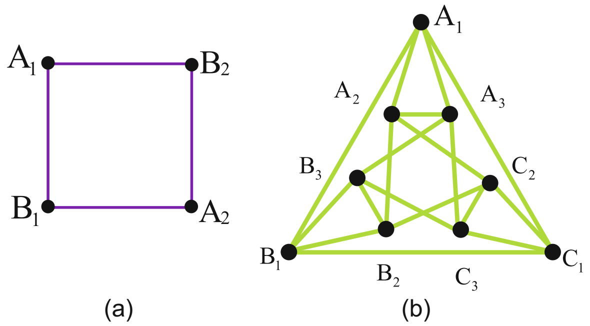

Fig. 1. Several typical compatibility graphs: (a) the Bell inequality [30,31], (b) the Peres-Mermin magical square [32].

fixed events. In that scenario, the events indicated by the vertices of the exclusivity graph are not fixed. Then an exclusivity graph may correspond to more than one compatibility graph.

Several sufficient conditions for exhibiting the quantum correlation in the compatibility-fixed scenario have already been shown in Figure 1, such as the Bell inequality [30,31] and the Peres-Mermin magical square [32,33]. In these cases, their corresponding compatibility graphs are all non-chordal. The chordal graph is a graph which hasn't any cycle with more than three vertices as its induced subgraph [27]. If a graph does not satisfy this condition, it is a non-chordal graph.

Result 1: The non-chordal compatibility graph is the sufficient condition for exhibiting quantum correlations in the compatibility-fixed (events-fixed) scenario.

Proof.

Due to the definition of the chordal graph, non-chordal graph G_c has an cycle consists of $\{A_{j_1}, \dots, A_{j_m}\}(m \geq 4)$ as its induce subgraph.

When m is odd, an inequality based on this cycle can be derived from the noncontextual hidden variable theory [29]:

$$\sum_{i=1}^{m-1} A_{j_i}A_{j_{i+1}} + A_{j_m}A_{j_1} \geq -m + 2. \quad (1)$$

It is impossible that all terms of $A_{j_i}A_{j_{i+1}}$ are equal to -1. The lower NCHV bound is $-m + 2$ when one term of $A_{j_i}A_{j_{i+1}}$ is equal to $+1$ while others are -1. For the case of $m = 5$, it is the KCBS inequality [5].

When m is even, another inequality based on this cycle can be derived from the noncontextual hidden variable theory [29]:

$$\sum_{i=1}^{m-1} A_{j_i}A_{j_{i+1}} - A_{j_m}A_{j_1} \leq m - 2. \quad (2)$$

It is impossible that $\{A_1A_2, \dots, A_{m-1}A_m, A_mA_1\}$ is equal to $\{+1, \dots, +1, -1\}$. The upper NCHV bound is $m - 2$ when each term is equal to $+1$. For the case of $m = 4$, it is the Bell inequality [30,31].

For equations (1) and (2), there are observable sets $\{A_1, \dots, A_n\}$ satisfying the compatibility relations indicated by the non-chordal graph G_c. However, they are violated in quantum theory. The observable sets can be constructed as follows.

An orthogonal representation of a graph is a set of unit vector $\{|v_i\rangle\}$ in a Euclidean space where $|v_i\rangle$ and $|v_j\rangle$ are orthogonal if vertex i and j are not adjacent [34,35]. Furthermore, the orthogonal representation is faithful if two vectors corresponding adjacent vertices are not orthogonal [36]. For any compatibility graph G_c, there exists a faithful orthogonal representation $\{|v_i\rangle\}$ of its complement [37]. Then, $\langle v_i|v_j\rangle = 0$ if and only if vertex i and j are adjacent in the compatibility graph G_c.

(a) m is odd

$\{|v_i\rangle\}$ is a faithful orthogonal representation of the complement of the compatibility graph G_c. The dimension of the space spanned by $\{|v_i\rangle\}$ is finite since the number of vertices in G_c is finite. The handle vector $|\varphi\rangle$ and $\{|u_i\rangle\}$ which is the orthogonal representation of the complement of the odd cycle C_m, can be constructed in the orthogonal space of $\{|v_i\rangle\}$, so that $\langle u_i|v_j\rangle = 0$ and $\langle \varphi|v_j\rangle = 0$ for any vertex i in the C_m and any vertex j in the G_c. There exists a handle $|\varphi\rangle$ and an orthogonal representation $\{u_{j_1}, \dots, u_{j_m}\}$ of the complement of C_m satisfying $\sum_{i=1}^{m} |\langle\varphi|u_{j_i}\rangle|^2 = \vartheta(C_m) = \frac{m\cos\frac{\pi}{m}}{1+\cos\frac{\pi}{m}}$ [34,35].
The observable set $\{A_k\}(1 \leq k \leq n)$ can be constructed as

$$A_k = \begin{cases} 2|v_k\rangle\langle v_k| - 1 & \text{vertex } k \notin C_m \\ 2|u_k\rangle\langle u_k| + 2|v_k\rangle\langle v_k| - 1 & \text{vertex } k \in C_m. \end{cases}$$

The compatibility relations among this observable set $\{A_k\}$ satisfy G_c, the detail derivation is shown in the Supplementary Material. However, equation (1) is violated under the state $|\varphi\rangle$ in quantum theory since the left part is $-4\frac{m\cos\frac{\pi}{m}}{1+\cos\frac{\pi}{m}} + m$, which is less than $-m + 2(m \geq 5)$. The detail derivation is shown in the Supplementary Material.

(b) m is even

$\{|v_i\rangle\}$ is a faithful orthogonal representation of the complement of the compatibility graph G_c. The dimension of the space spanned by $\{|v_i\rangle\}$ is finite since the number of vertices in G_c is finite. One can find a four dimension space orthogonal to $\{|v_i\rangle\}$. The orthogonal bases of this space are four unit vectors $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$. In this space, $\{w_{j_i}\}$ and $\{z_{j_i}\}$ are constructed as:

$$|w_{j_i}\rangle = \begin{cases} \cos(i\frac{\pi}{2m})|1\rangle + \sin(i\frac{\pi}{2m})|2\rangle & i \text{ is odd} \\ \cos(i\frac{\pi}{2m})|1\rangle + \sin(i\frac{\pi}{2m})|3\rangle & i \text{ is even} \end{cases}$$

$$|z_{j_i}\rangle = \begin{cases} \cos(i\frac{\pi}{2m})|3\rangle + \sin(i\frac{\pi}{2m})|4\rangle & i \text{ is odd} \\ \cos(i\frac{\pi}{2m})|2\rangle + \sin(i\frac{\pi}{2m})|4\rangle & i \text{ is even.} \end{cases}$$

With the definitions of $\{w_{j_i}\}$ and $\{z_{j_i}\}$, an observable set $\{A_k\}(1 \leq k \leq n)$, can be constructed as

$$A_k = \begin{cases} 2|v_k\rangle\langle v_k| - 1 & \text{vertex } k \notin C_m \\ 2|w_k\rangle\langle w_k| + 2|z_k\rangle\langle z_k| + 2|v_k\rangle\langle v_k| - 1 & \\ & \text{vertex } k \in C_m. \end{cases}$$

The compatibility relations among this observable set $\{A_k\}$, satisfy G_c, the detail derivation is shown in the Supplementary Material. However, equation (2) is violated under the state of $|\varphi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |4\rangle)$ in quantum theory since the left part is $m \cos\frac{\pi}{m}$, which is larger than $m-2\,(m \geq 4)$. The detail derivation is shown in the Supplementary Material.

In the proof of the Result 1, if one only constructs the observable set $\{A_{j_1}, \ldots, A_{j_m}\}$ on the cycle which leads the violation of equation (1) (or Eq. (2)), it can't prove the non-chordal compatibility graph can exhibit the quantum correlations since there may not exist the observables out of the cycle under the constraints of the compatibility relations. It is necessary to prove the existence of all observables after constructing the NC inequality which is violated in quantum mechanics.

Corollary 1. The non-chordal compatibility graph is the necessary and sufficient condition for exhibiting quantum correlations in the compatibility-fixed (events-fixed) scenario.

Proof. It is shown that if the compatibility graph is a chordal graph, for each observable set satisfying the graph, there exists the joint probability distribution which recovers the probability distributions of any joint measurable subset as marginal [27]. With the Result 1, the non-chordal compatibility graph is the necessary and sufficient condition in the compatibility-fixed (events-fixed) scenario.

The contextuality is revealed by the violation of non-contextuality inequalities [20–26]. The classical bound of a non-contextuality inequality is the independence number of its exclusivity graph, which is the cardinality of the largest independent vertex set and is commonly denoted by $\alpha(G)$, while the quantum bound can be obtained by the semi-definite program [23]. In the scenario discussed in reference [23], the quantum bound is the Lovász number which is a real number, representing an upper bound on the Shannon capacity of the graph, and is commonly denoted by $\vartheta(G)$. Hence the classical bound is equal to the quantum bound while the exclusivity graph is perfect. The perfect graph is a graph which hasn't any odd cycle or odd cycle's complement with more than four vertices as its induced subgraph [23]. If a graph does not satisfy this condition, it is an imperfect graph. As a result, the imperfect exclusivity graph is the necessary and sufficient condition for exhibiting quantum correlations in that scenario where the events indicated by the vertices of the exclusivity graph are not fixed. However, in the events-fixed (compatibility-fixed) scenario we discussed here, the events indicated by the vertices of the exclusivity graph are fixed. Hence, the NCHV inequality may not reach the Lovász number [38].

Result 2: The imperfect exclusivity graph is not a sufficient condition for exhibiting quantum correlations in the events-fixed (compatibility-fixed) scenario.

Proof.

In the events-fixed (compatibility-fixed) scenario, we show an example in Figure 2. An exclusivity graph is shown in Figure 2a. $\{A_1,\ A_2,\ A_6\}$, $\{A_2,\ A_3,\ A_7\}$,

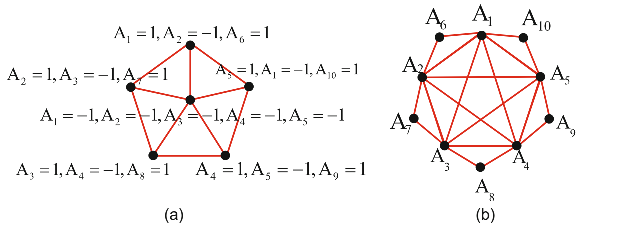

Fig. 2. (a) The exclusivity graph of the observable set $\{A_1, \ldots, A_{10}\}$. (b) The compatibility graph of an observable set $\{A_1, \ldots, A_{10}\}$.

$\{A_3,\ A_4,\ A_8\}$, $\{A_4,\ A_5,\ A_9\}$, $\{A_5,\ A_1,\ A_{10}\}$ and $\{A_1,\ A_2,\ A_3,\ A_4,\ A_5\}$ are jointly measurable observable sets. From these compatibility relations among the observables, the corresponding compatibility graph of observables $\{A_1, \ldots, A_{10}\}$ is shown in Figure 2b. On the other hand, an induced subgraph of the exclusivity graph Figure 2a is a pentagon consisting of five events $\{(A_1 = 1, A_2 = -1, A_6 = 1), (A_2 = 1, A_3 = -1, A_7 = 1), (A_3 = 1, A_4 = -1, A_8 = 1), (A_4 = 1, A_5 = -1, A_9 = 1), (A_5 = 1, A_1 = -1, A_{10} = 1)\}$. The exclusivity graph is a imperfect graph since it has a pentagon as its induce subgraph [41]. However, due to the Corollary 1, the joint probability distribution of these observables can be constructed as

$$P(A_1 = a_1, \ldots, A_{10} = a_{10}) = P(A_1 = a_1, \ldots, A_5 = a_5) \times \prod_{i=1}^{5} \frac{P(A_i = a_i, A_{i+1(mod5)} = a_{i+1(mod5)}, A_{i+5} = a_{i+5})}{P(A_i = a_i, A_{i+1(mod5)} = a_{i+1(mod5)})}$$

since Figure 2a is a chordal graph [27]. As a result, the observable set $\{A_1, \ldots, A_{10}\}$ cannot exhibit quantum correlations. It can be concluded that there are imperfect exclusivity graphs, which can't exhibit quantum correlations in the events-fixed (compatibility-fixed) scenario.

In the example for the proof of no sufficiency in the Result 2, the non-contextuality inequality of the five events shown in Figure 2b is

$$\sum_{i=1}^{5} P(A_i = 1, A_{i+1} = -1, A_{i+5} = 1) \leq \alpha(C_5) = 2 \quad (3)$$

$$\sum_{i=1}^{5} P(A_i = 1, A_{i+1} = -1, A_{i+5} = 1) \leq 2. \quad (4)$$

Although the exclusivity graph of the five events in Figure 2 is a pentagon, the quantum bound of the inequality can't reach $\vartheta(C_5) = \sqrt{5}$ since there doesn't exist any observable set satisfying the following two conditions simultaneously: (i) the compatibility relations among these observables satisfy Figure 2a; (ii) the probabilities of the events $P(A_i = 1, A_{i+1} = -1, A_{i+5} = 1)$ $(1 \leq i \leq 5)$ are equal to $|\langle\phi|v_i\rangle|^2$ $(1 \leq i \leq 5)$, where $|\phi\rangle$ is the handle, $|v_i\rangle$ is the orthogonal representation of a pentagon and $\sum_{i=1}^{5} |\langle\phi|v_i\rangle|^2 = \vartheta(C_5)$.

For the case in reference [38], the quantum bound cannot reach $\vartheta(C_5)$ but is still larger than $\alpha(C_5)$. It means

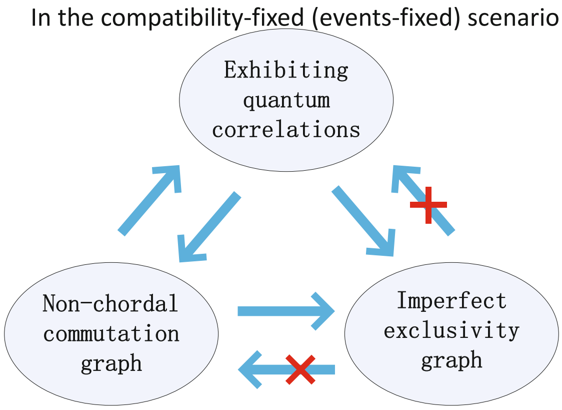

Fig. 3. The relations among the compatibility graph, exclusivity graph and exhibiting quantum correlations in the compatibility-fixed (events-fixed) scenario.

that quantum correlations can be singled out. However, for the observable sets satisfying Figure 2, the quantum bound is also not reach the $\vartheta(C_5)$. Furthermore, the quantum bound of equation (4) is equal to the NCHV bound.

Corollary 2. The imperfect compatibility graph is the necessary but not sufficient condition for exhibiting quantum correlations in the events-fixed (compatibility-fixed) scenario.

Proof. It is shown that if the exclusivity graph is a perfect graph, the probabilistic $p = (p_1, \ldots, p_i, \ldots, p_k)$ (p_i denotes the probability of event corresponding the vertex i) constructs a convex hull of several deterministic model. Since the graph theory result that $STAB(G) = QSTAB(G)$ [39,40], the probability can be expressed by the noncontextual hidden variable model. This is proved in reference [24]. With the Result 2, the imperfect compatibility graph is the necessary but not sufficient condition in the events-fixed (compatibility-fixed) scenario.

The relation between the non-chordal compatibility graph and exhibiting quantum correlations in the compatibility-fixed (events-fixed) scenario is shown in Corollary 1. The relation between the imperfect exclusivity graph and exhibiting quantum correlations in the events-fixed (compatibility-fixed) scenario is shown in Corollary 2. The relations are summarized in Figure 3.

Conclusion. We show the non-chordal compatibility graph can construct a non-contextuality inequality which is violated in quantum theory in the compatibility-fixed (events-fixed) scenario. It infers that the non-chordal compatibility graph is a sufficient condition for exhibiting quantum correlations in the compatibility-fixed (events-fixed) scenario. We also display an example to show a specific imperfect exclusivity graph which admits the joint probability distribution in the events-fixed (compatibility-fixed) scenario. It infers that the imperfect exclusivity graph is an insufficient condition for exhibiting quantum correlations in the events-fixed (compatibility-fixed) scenario. This result provides a convenient tool to determine whether an observable set can single out the quantum correlation in the compatibility-fixed (events-fixed) scenario, which is important in investigations on quantum contextuality.

Authors contributions and statement

F.Z. toke the theoretical analysis and wrote the manuscript. W.Z. checked the theoretical results and wrote the manuscript. Y.D.H. supervised the project and edited the manuscript.

This work was supported by 973 Programs of China under Contract No. 2011CBA00303 and 2013CB328700, Basic Research Foundation of Tsinghua National Laboratory for Information Science and Technology (TNList).

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