On the Djoković–Winkler Relation and Its Closure in Subdivisions of Fullerenes, Triangulations, and Chordal Graphs

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Abstract

It was recently pointed out that certain SiO\textsubscript{2} layer structures and SiO\textsubscript{2} nanotubes can be described as full subdivisions aka subdivision graphs of partial cubes. A key tool for analyzing distance-based topological indices in molecular graphs is the Djoković-Winkler relation $\Theta$ and its transitive closure $\Theta^*$. In this paper we study the behavior of $\Theta$ and $\Theta^*$ with respect to full subdivisions. We apply our results to describe $\Theta^*$ in full subdivisions of fullerenes, plane triangulations, and chordal graphs.

1 Introduction

Partial cubes, that is, graphs that admit isometric embeddings into hypercubes, are of great interest in metric graph theory. Fundamental results on partial cubes are due to Chepoi \cite{Chepoi}, Djoković \cite{Djokovic}, and Winkler \cite{Winkler}. The original source for their interest however goes back to the paper of Graham and Pollak \cite{GrahamPollak}. For additional information on partial
cubes we refer to the books [12, 16], the semi-survey [26], recent papers [1, 7, 24], as well as references therein.

Partial cubes offer many applications, ranging from the original one in interconnection networks [18] to media theory [16]. Our motivation though comes from mathematical chemistry where many important classes of chemical graphs are partial cubes. In the seminal paper [21] it was shown that the celebrated Wiener index of a partial cube can be obtained without actually computing the distance between all pairs of vertices. A decade later it was proved in [20], based on the Graham-Winkler’s canonical metric embedding [19], that the method extends to arbitrary graphs. The paper [21] initiated the theory under the common name “cut method,” while [23] surveys the results on the method until 2015 with 97 papers in the bibliography. The cut method has been further developed afterwards, see [6, 9, 25, 30, 31] for some recent results on it related to partial cubes.

Now, in a series of papers [3–5] it was observed that certain SiO$_2$ layer structures and SiO$_2$ nanotubes that are of importance in chemistry can be described as the full subdivisions aka subdivision graphs of relatively simple partial cubes. (The paper [29] can serve as a possible starting point for the role of SiO$_2$ nanostructures in chemistry.) The key step of the cut-method for distance based (as well as some other) invariants is to understand and compute the relation $\Theta^*$. Therefore in [4] it was proved that the $\Theta^*$-classes of the full subdivision of a partial cube $G$ can be obtained from the $\Theta^*$-classes of $G$. Note that in a partial cube the latter coincide with the $\Theta$-classes.

The above developments yield the following natural, general problem that intrigued us: Given a graph $G$ and its $\Theta^*$-classes, determine the $\Theta^*$-classes of the full subdivision of $G$. In this paper we study this problem and prove several general results that can be applied in cases such as in [3–5] in mathematical chemistry as well as elsewhere. In the next section we list known facts about the relations $\Theta$ and $\Theta^*$ as well as the distance function in full subdivisions needed in the rest of the paper. In Section 3, general properties of the relations $\Theta$ and $\Theta^*$ in full subdivisions are derived. These properties are then applied in the subsequent sections. In the first of them, $\Theta^*$ is described for fullerenes (a central class of chemical graph theory, see e.g. [2, 15, 17, 27, 28, 33, 34]) and plane triangulations. In Section 5 the same problem is solved for chordal graphs.
2 Preliminaries

If $R$ is a relation, then $R^*$ denotes its transitive closure. The distance $d_G(x, y)$ between vertices $x$ and $y$ of a connected graph $G$ is the usual shortest path distance. If $x \in V(G)$ and $e = \{y, z\} \in E(G)$, then let

$$d_G(x, e) = \min\{d_G(x, y), d_G(x, z)\}.$$  

Similarly, if $e = \{x, y\} \in E(G)$ and $f = \{u, v\} \in E(G)$, then we set

$$d_G(e, f) = \min\{d_G(x, u), d_G(x, v), d_G(y, u), d_G(y, v)\}.$$  

Note that the latter function does not yield a metric space because if $e$ and $f$ are adjacent edges then $d_G(e, f) = 0$. To get a metric space, one can define the distance between edges as the distance between the corresponding vertices in the line graph of $G$. But for our purposes the function $d_G(e, f)$ as defined is more suitable.

Edges $e = \{x, y\}$ and $f = \{u, v\}$ of a graph $G$ are in relation $\Theta$, shortly $e \Theta f$, if $d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u)$. If $G$ is bipartite, then the definition simplifies as follows.

**Lemma 2.1** If $e = \{x, y\}$ and $f = \{u, v\}$ are edges of a bipartite graph $G$ with $e \Theta f$, then the notation can be chosen such that $d_G(u, x) = d_G(v, y) = d_G(u, y) = d_G(v, x) = 1$.

The relation $\Theta$ is reflexive and symmetric. Hence $\Theta^*$ is an equivalence relation, its classes are called $\Theta^*$-classes. Partial cubes are precisely those connected bipartite graph for which $\Theta = \Theta^*$ holds [32]. In partial cubes we may thus speak of $\Theta$-classes instead of $\Theta^*$-classes. In the following lemma we collect properties of $\Theta$ to be implicitly or explicitly used later on.

**Lemma 2.2** (i) If $P$ is a shortest path in $G$, then no two distinct edges of $P$ are in relation $\Theta$.

(ii) If $e$ and $f$ are edges from different blocks of a graph $G$, then $e$ is not in relation $\Theta$ with $f$.

(iii) If $e$ and $f$ are edges of an isometric cycle $C$ of a bipartite graph $G$, then $e \Theta f$ if and only if $e$ and $f$ are antipodal edges of $C$. 

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(iv) If $H$ is an isometric subgraph of a graph $G$, then $\Theta_H$ is the restriction of $\Theta_G$ to $H$.

If $G$ is a graph, then the graph obtained from $G$ by subdividing each edge of $G$ exactly once is called the full subdivision (graph) of $G$ and denoted with $S(G)$. We will use the following related notation. If $x \in V(G)$ and $e = \{x, y\} \in E(G)$, then the vertex of $S(G)$ corresponding to $x$ will be denoted by $\bar{x}$ and the vertex of $S(G)$ obtained by subdividing the edge $e$ with $xy$. Two edges incident with $xy$ will be denoted with $e_{\bar{x}}$ and $e_{\bar{y}}$, where $e_{\bar{x}} = \{\bar{x}, \overline{xy}\}$ and $e_{\bar{y}} = \{\bar{y}, \overline{xy}\}$. See Fig. 1 for an illustration.

**Figure 1.** Notation for the vertices and edges of $S(G)$.

The following lemma is straightforward, cf. [22, Lemma 2.3].

**Lemma 2.3** If $G$ is a connected graph, then the following assertions hold.

(i) If $x, y \in V(G)$, then $d_{S(G)}(\bar{x}, \bar{y}) = 2d_G(x, y)$.

(ii) If $x \in V(G)$ and $\{y, z\} \in E(G)$, then $d_{S(G)}(\bar{x}, \overline{yz}) = 2d_G(x, \{y, z\}) + 1$.

(iii) If $\{x, y\}, \{u, v\} \in E(G)$, then $d_{S(G)}(\overline{xy}, \overline{uv}) = 2d_G(\{x, y\}, \{u, v\}) + 2$.

### 3 $\Theta^*$ in full subdivisions

**Lemma 3.1** If $G$ is a connected graph and $e_{\bar{x}} \Theta_{S(G)} f_{\bar{u}}$, then $e \Theta_G f$.

**Proof.** Let $e = \{x, y\}$ and $f = \{u, v\}$. If $\bar{x} = \bar{u}$ and $\bar{y} = \bar{v}$, then $e_{\bar{x}} = f_{\bar{u}}$ and $e = f$, so there is nothing to prove. If $\bar{x} = \bar{v}$ and $\bar{y} = \bar{u}$, then $e_{\bar{x}}$ and $f_{\bar{u}}$ are adjacent edges which cannot be in relation $\Theta_{S(G)}$ because $S(G)$ is triangle-free. For the same reason the situation $\bar{x} = \bar{u}$ and $\bar{y} \neq \bar{v}$ is not possible. Assume next that $\bar{x} = \bar{v}$ and $\bar{y} \neq \bar{u}$. Then $d_{S(G)}(\bar{u}, \overline{xy}) = 3$ by Lemma 2.3, and hence $\overline{xy}, \overline{uv}, \bar{u}$ is a geodesic containing $e_{\bar{x}}$ and $f_{\bar{u}}$, contradiction the assumption $e_{\bar{x}} \Theta_{S(G)} f_{\bar{u}}$. In the rest of the proof we may thus assume that $\{x, y\} \cap \{u, v\} = \emptyset$. 


Since $S(G)$ is bipartite, in view of Lemma 2.1 we need to consider the following two cases, where, using Lemma 2.3(i), we can assume that the distances $d_{S(G)}(x, ar{u})$ and $d_{S(G)}(xy, ar{w})$ are even. Based on the assumption $e_\varepsilon \varTheta_{S(G)}f_\bar{u}$, we have $d_{S(G)}(x, ar{u}) + d_{S(G)}(xy, \bar{w}) = d_{S(G)}(x, \bar{w}) + d_{S(G)}(xy, \bar{u})$ in a bipartite graph, thus the following cases.

**Case 1.** $d_{S(G)}(x, \bar{u}) = d_{S(G)}(xy, \bar{w}) = 2k$ and $d_{S(G)}(x, \bar{w}) = d_{S(G)}(xy, \bar{u}) = 2k + 1$.

In the following, Lemma 2.3 will be used all the time.

By $2k = d_{S(G)}(xy, \bar{w}) = 2d_G(\{x, y\}, \{u, v\}) + 2$, we get

$$k - 1 \leq d_G(y, v), d_G(x, u), d_G(x, v), d_G(y, u),$$

where the lower bound is attained at least once.

Since $d_{S(G)}(x, \bar{u}) = 2k$, we have $d_G(x, u) = k$. Because $d_{S(G)}(\bar{x}, \bar{w}) = 2k + 1$, we find that $d_G(x, \{u, v\}) = k$ and hence in particular $d_G(x, v) \geq k$. Similarly, as $d_{S(G)}(xy, \bar{u}) = 2k + 1$ we have $d_G(u, \{x, y\}) = k$ and hence in particular $d_G(u, y) \geq k$. With the first observation this yields $k - 1 = d_G(y, v)$. In summary,

$$d_G(x, u) + d_G(y, v) = k + (k - 1) \neq k + k \leq d_G(x, v) + d_G(y, u),$$

which means that $e \varTheta_{G}f$.

**Case 2.** $d_{S(G)}(x, \bar{u}) = d_{S(G)}(xy, \bar{w}) = 2k$ and $d_{S(G)}(\bar{x}, \bar{w}) = d_{S(G)}(xy, \bar{u}) = 2k - 1$.

Again, $d_{S(G)}(x, \bar{u}) = 2k$ implies $d_G(x, u) = k$. The assumption $d_{S(G)}(x, \bar{w}) = 2k - 1$ yields $d_G(x, \{u, v\}) = k - 1$ and consequently $d_G(x, v) = k - 1$. The condition $d_{S(G)}(xy, \bar{u}) = 2k - 1$ implies $d_G(u, \{x, y\}) = k - 1$ and so $d_G(u, y) = k - 1$. Finally, the assumption $d_{S(G)}(xy, \bar{w}) = 2k$ gives us $d_G(\{x, y\}, \{u, v\}) = k - 1$, in particular, $d_G(y, v) \geq k - 1$.

Putting these facts together we get

$$d_G(x, u) + d_G(y, v) \geq k + (k - 1) > (k - 1) + (k - 1) = d_G(x, v) + d_G(y, u),$$

hence again $e \varTheta_{G}f$.

Lemma 3.1 implies the following result on the relation $\varTheta^*$.

**Corollary 3.2** If $e_\varepsilon \varTheta^*_{S(G)}f_\bar{u}$, then $e\varTheta^*_{G}f$.

**Proof.** Suppose $e_\varepsilon \varTheta^*_{S(G)}f_\bar{u}$. Then there exists a positive integer $k$ such that

$$e_\varepsilon \varTheta_{S(G)}f_{\bar{u}}^{(1)} = f_{\bar{u}}^{(1)} \varTheta_{S(G)}f_{\bar{u}}^{(2)} = \ldots = f_{\bar{u}}^{(k)} \varTheta_{S(G)}f_{\bar{u}}.$$


Then, by Lemma 3.1, we have
\[ e \Theta_G f^{(1)}, f^{(1)} \Theta_G f^{(2)}, \ldots, f^{(k)} \Theta_G f, \]
implying that \( e \Theta_G f. \)

The next lemma is a partial converse to Lemma 3.1.

**Lemma 3.3** If \( e \Theta_G f, \) then there is a pair of edges \( e_x, f_u \) in \( S(G) \) such that \( e_x \Theta_{S(G)} f_u. \) Moreover, if \( G \) is bipartite, then there are two (disjoint) such pairs.

**Proof.** Let \( e = \{x, y\}, f = \{u, v\}, \) and let \( k = d_G(x, u). \) Since \( e \Theta_G f, \) we may without loss of generality assume that \( d_G(x, u) + d_G(y, v) < d_G(y, u) + d_G(x, v) \) and that \( d_G(x, u) \leq d_G(y, v). \) We distinguish the following cases.

**Case 1.** \( d_G(y, v) = k. \)

In this case, \( \{d_G(x, v), d_G(y, u)\} \subseteq \{k - 1, k, k + 1\}. \) Moreover, our assumption about the sum of distances implies that \( \{d_G(x, v), d_G(y, u)\} \subseteq \{k, k + 1\}. \) Since \( e \Theta_G f, \) the two distances cannot both be equal to \( k. \) Hence, up to symmetry, we need to consider the following two subcases.

Suppose \( d_G(x, v) = d_G(y, u) = k + 1. \) Then \( d_{S(G)}(\bar{x}, \bar{v}) = 2k + 2, d_{S(G)}(\bar{x}y, \bar{w}) = 2k + 2, d_{S(G)}(\bar{x}, \bar{w}) = 2k + 1, \) and \( d_{S(G)}(\bar{y} \bar{y}, \bar{v}) = 2k + 1. \) Hence \( e_x \Theta_{S(G)} f_{\bar{u}}. \)

Suppose \( d_G(x, v) = k \) and \( d_G(y, u) = k + 1. \) Then \( d_{S(G)}(\bar{y}, \bar{u}) = 2k + 2, d_{S(G)}(\bar{y} \bar{y}, \bar{w}) = 2k + 2, d_{S(G)}(\bar{y}, \bar{w}) = 2k + 1, \) and \( d_{S(G)}(\bar{x} \bar{y}, \bar{u}) = 2k + 1. \) Hence \( e_y \Theta_{S(G)} f_{\bar{u}}. \) A similar situation occurs when \( d_G(x, v) = k + 1 \) and \( d_G(y, u) = k. \)

**Case 2.** \( d_G(y, v) = k + 1. \)

Again, \( \{d_G(x, v), d_G(y, u)\} \subseteq \{k - 1, k, k + 1\}, \) but since \( d_G(x, u) + d_G(y, v) < d_G(y, u) + d_G(x, v) \) it must be that \( d_G(x, v) = d_G(y, u) = k + 1. \) Then \( d_{S(G)}(\bar{y}, \bar{v}) = 2k + 2, d_{S(G)}(\bar{x} \bar{y}, \bar{w}) = 2k + 2, d_{S(G)}(\bar{y} \bar{w}) = 2k + 3, \) and \( d_{S(G)}(\bar{x} \bar{y}, \bar{v}) = 2k + 3. \) Hence \( e_y \Theta_{S(G)} f_{\bar{u}}. \)

**Case 3.** \( d_G(y, v) = k + 2. \)

In this case the fact that \( \{d_G(x, v), d_G(y, u)\} \subseteq \{k - 1, k, k + 1\} \) implies that \( d_G(x, u) + d_G(y, v) \geq d_G(y, u) + d_G(x, v). \) As this is not possible, the first assertion of the lemma is proved.

Assume now that \( G \) is bipartite. Combining Lemma 2.1 with the above case analysis we infer that the only case to consider is when \( d_G(x, u) = d_G(y, v) = k \) and \( d_G(x, v) = d_G(y, u) = k + 1. \) Then, just in the first subcase of the above Case 1 we get that \( e_x \Theta_{S(G)} f_{\bar{u}} \) and, similarly, \( e_y \Theta_{S(G)} f_{\bar{u}}. \)
We say that cycles $C$ and $C'$ of $G$ are *isometrically touching* if $|E(C) \cap E(C')| = 1$ and $C \cup C'$ is an isometric subgraph of $G$. Note that isometrically touching cycles are isometric.

**Figure 2.** Isometrically touching cycles and their subdivisions.

**Lemma 3.4** Let $C$ and $C'$ be isometrically touching cycles in $G$ with $E(C) \cap E(C') = \{e\}$. Then in $S(G)$ both edges corresponding to $e$ are in the same $\Theta_{S(G)}^*$-class. Moreover, this class contains the edges thickened in Fig. 2.

**Proof.** We take the notation from Fig. 2 and content ourselves with only providing the proof for the case where $C$ is odd and $C'$ is even. The other cases go through similarly. From Lemma 2.2(iii) we get that $\{\overline{u}, \overline{uv}\} \Theta_{S(G)} \{\overline{w}, \overline{tw}\}$ and $\{\overline{u}, \overline{uw}\} \Theta_{S(G)} \{\overline{y}, \overline{xy}\}$. However, note now that $d(\overline{y}, \overline{w}) = d(\overline{xy}, \overline{sw}) = d(\overline{y}, \overline{sw}) - 1 = d(\overline{xy}, \overline{w}) - 1$. Thus we also have $\{\overline{w}, \overline{sw}\} \Theta_{S(G)} \{\overline{y}, \overline{xy}\}$. Since $\{\overline{w}, \overline{sw}\}$ is also in relation with $\{\overline{v}, \overline{uv}\}$ we obtain the claim for $\Theta_{S(G)}^*$ by taking the transitive closure. □

For the full subdivision $S(G)$ of $G$ denote by $S(\Theta_{G}^*)$, the relation on the edges of $S(G)$, where $\{\overline{x}, \overline{xy}\}$ and $\{\overline{u}, \overline{uv}\}$ are in relation $S(\Theta_{G}^*)$ if and only if $\{x, y\} \Theta^* \{u, v\}$. In particular, $\{\overline{x}, \overline{xy}\}$ and $\{\overline{xy}, \overline{y}\}$ are always in relation.

**Lemma 3.5** We have $\{\overline{x}, \overline{xy}\} \Theta_{S(G)}^* \{\overline{xy}, \overline{y}\}$ for all $\{x, y\} \in G$ if and only if $\Theta_{S(G)}^* = S(\Theta_{G}^*)$. 
Proof. The backwards direction holds by definition. Conversely, by Lemma 3.1 we have that if \( \{\bar{x}, \bar{y}\} \Theta^*_{S(G)} \{\bar{w}, \bar{v}\} \), then \( \{x, y\} \Theta^* \{u, v\} \). Therefore, \( \Theta^*_{S(G)} \subseteq S(\Theta^*_G) \). On the other hand, Lemma 3.3 assures that if \( \{x, y\} \Theta^* \{u, v\} \), then there is a pair \( \{\bar{x}, \bar{y}\} \Theta^*_{S(G)} \{\bar{w}, \bar{v}\} \), but then by our assumption also \( \{\bar{y}, \bar{y}\} \Theta^*_{S(G)} \{\bar{w}, \bar{v}\} \) and so on. Thus, \( \Theta^*_{S(G)} \supseteq S(\Theta^*_G) \).

Lemma 3.4 and 3.5 immediately yield:

Proposition 3.6 If every edge of \( G \) is in the intersection of two isometrically touching cycles, then \( \Theta^*_{S(G)} = S(\Theta^*_G) \).

4 \( \Theta^* \) in subdivisions of fullerenes and plane triangulations

In this section we study relation \( \Theta^* \) in full subdivisions of fullerenes and plane triangulations, for which Proposition 3.6 will be essential. We begin with fullerenes. Recall that a fullerene is a 3-connected, cubic, planar graph all of whose faces are of length 5 or 6.

A cycle \( C \) of a connected graph \( G \) is separating if \( G \setminus C \) is disconnected. A cyclic edge-cut of \( G \) is an edge set \( F \) such that \( G \setminus F \) separates two cycles. To prove our main result on fullerenes we need the following result.

Lemma 4.1 Given a fullerene graph \( G \), every separating cycle of \( G \) is of length at least 9. Moreover, the only separating cycles of length 9, are the cycles separating a vertex incident only to 5-faces, see the left of Fig. 3.

Proof. Let \( C \) be a separating cycle of length at most 9. Since \( G \) is cubic, there are \( |C| \) edges of \( G \) incident to \( C \) which are not in \( C \). Thus, without loss of generality, we may assume at most four of them are in the inner side of \( C \). As they form an edge cut, and since fullerenes are cyclically 5-edge-connected [14], the subgraph induced by vertices in the inner part of \( C \) is a forest, say \( F \). If \( F \) consists of one vertex, say \( v \), then we have three edges connecting \( v \) to \( C \) which form three faces \( G \). As each of these faces is of length at least 5, they are exactly 5-faces. Otherwise, \( F \) contains at least two vertices \( u \) and \( v \) each of which is either an isolated vertex of \( F \) or a leaf. As they are of degree 3 in \( F \), each of them must be connected by two edges to \( C \). And since there at most four such edges, it follows that \( u \) and \( v \) are of degree 1 in \( F \) and that every other vertex of \( F \) is of degree 3 in \( F \), which means there no other vertex and \( u \) is adjacent to \( v \). Thus inside \( C \) we have
five edges and four faces. But $C$ itself is of length at most 9 and thus one of these four faces is of length at most 4, a contradiction with the choice of $G$.

Figure 3. A separating 9-cycle and isometrically touching 6-cycles.

**Theorem 4.2** If $G$ is a fullerene, then $\Theta^e_S(G) = S(\Theta^e_S(G))$.

**Proof.** We claim that every edge $e$ of $G$ is the intersection of two isometrically touching cycles. For this sake consider the cycles $C$ and $C'$ that lie on the boundary of the faces containing $e$. We have to prove that the union $C \cup C'$ is isometric. Assume on the contrary that this is not the case, that is, there exist vertices $u, v \in C \cup C'$ such that there is a shortest $u, v$-path $P$ (in $G$) interiorly disjoint from $C \cup C'$, that is shorter than any shortest path $P'$ from $u$ to $v$ in $C \cup C'$.

Consider the cycle $C''$ obtained by joining $P$ and a shortest path $P'$ from $u$ to $v$ in $C \cup C'$. Since $C$ and $C'$ are of length at most 6, the graph $C \cup C'$ is of diameter at most 5, thus the cycle $C''$ is of length at most 9. We will prove that there is a separating cycle contradicting Lemma 4.1.

First, note that if $e \in P'$, then $C''$ separates the graph $C \cup C'$. Thus, by Lemma 4.1 $C''$ is of length at most 9, so the endpoints of $P'$ must be at distance 5 on $C \cup C'$, i.e., one is in $C$ and the other in $C'$. Thus, both sides of $C''$ contain more than one vertex, contradicting Lemma 4.1.

Hence, $P'$ is on the boundary of $C \cup C'$. Suppose that $C''$ is not induced. Then since the girth of fullerenes is 5, there is a single chord from $P$ to $P'$ which splits $C''$ into a 5-cycle $A$ and into a 5- or a 6-cycle $B$. In particular, $|C''| \geq 8$ and $P'$ has at least five vertices on $C''$. Thus, one vertex of $P'$ has degree 2 in $C \cup C'$ and is not incident to the
chord. Thus, this vertex has a neighbor in the interior of $A$ or $B$, that is, one of them is separating, contradicting Lemma 4.1.

If $C''$ is induced, it follows from the fact that $C$ and $C'$ are faces and $|C''| \geq 5$, that $C''$ is not a face, i.e., it is separating. Thus, $|C''| = 9$ and the patch $Q$ consisting of $C''$ and its interior is a single vertex surrounded by three 5-faces, see Lemma 4.1. Moreover, $C$ and $C'$ are 6-faces so that their union can have diameter 5. Note that any path $P'$ on the boundary of $C \cup C''$ of length 5 uses only one vertex of degree 3, see the right of Fig. 3. But any path $P'$ of length 5 on the boundary $Q$ uses at least two vertices of degree 2, see the left of Fig. 3. Thus, $P'$ cannot be in both boundaries simultaneously – contradiction.

We have shown the claim from the beginning and Proposition 3.6 yields the result.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{A fullerene $G$ which has two $\Phi^*$-classes (bold and normal edges), but only one $\Theta^*_G$-class since $e\Theta_G f$.}
\end{figure}

We have proved how $\Theta^*_G$ of a fullerene behaves with respect to subdivision. What can we say about $\Theta^*_G$ itself? If $G$ is a fullerene, then we define a relation $\Phi$ on $E(G)$ as follows: $e\Phi f$ if $e$ and $f$ are opposite edges of a facial $C_6$. Relation $\Phi$ falls into cycles and paths, that have been called \textit{railroads} [11]. In particular, it has been shown that cycles
can have multiple self-intersection. We denote by $\Phi$ the relation where additionally any two non-incident edges of a facial $C_5$ are in relation. Finally, recall that $\Phi^*$ denotes the transitive closure of $\Phi$. Since faces are isometric subgraphs, it is easy to see that $\Phi$ is a refinement of $\Theta_G$ as well as $\Phi^*$ is a refinement of $\Theta^*_G$. One might believe that the converse also holds, but the example in Fig. 4 shows that this is not always the case. We believe that determining $\Theta^*_G$ in fullerenes is an interesting problem.

We now turn our attention to plane triangulations. It is straightforward to verify that if $G$ is a plane triangulation, then $\Theta^*$ consists of a single class. On the other hand, $\Theta^*$ on the full subdivision of a plane triangulation has the following non-trivial structure.

Theorem 4.3 Let $G \neq K_4$ be a plane triangulation. Then $\Theta^*_S(G)$ consists of one global class $\gamma$, plus one class $\gamma_x$ for every degree three vertex $x$. Here, if $N(x) = \{y_1, y_2, y_3\}$, then $\gamma_x = \{\{\bar{y}_1, y_1x\}, \{\bar{y}_2, y_2x\}, \{\bar{y}_3, y_3x\}\}$. If $G = K_4$ the same holds, except that there is no global class $\gamma$.

Proof. Recall that $S(K_4)$ is a partial cube, cf. [22], its $\Theta$-classes (:= $\Theta^*$-classes) are shown in Fig. 5. Hence the result holds for $K_4$.

![Figure 5. The relation $\Theta^*$ in $S(K_4)$ and the full division of the graph obtained by stacking into one face.](image)

We proceed by induction on the number of vertices. Let $G$ have minimum degree at least 4, and let $e = \{x, y\}$ be an edge shared by triangles $C$ and $C'$ bonding faces of $G$. If $C \cup C'$ is isometric, then by Lemma 3.4 we have $\{\bar{x}, xy\} \Theta^*_{S(G)} \{\bar{y}, y\}$. Otherwise, $C \cup C'$ induces a $K_4$, but since the minimum degree of $G$ is at least 4, the other two triangles of the $K_4$ cannot be faces. An easy application of Lemma 3.4 on the other edges of this $K_4$ implies $\{\bar{x}, xy\} \Theta^*_{S(G)} \{\bar{y}, y\}$. Since in a triangulation there is only one $\Theta^*$-class, Proposition 3.6 implies the result, that is, there is only one global class $\gamma$ in $S(G)$.
Now suppose that $G$ contains a vertex $v$ of degree 3. The graph $G' = G \setminus \{v\}$ is a plane triangulation, thus our claim holds for $G'$ by induction. In particular, if $G' = K_4$, see Fig. 5 again. Otherwise, since $S(G')$ is an isometric subgraph of $S(G)$, Lemma 2.2(iv) says that $\Theta_{S(G')}^*$ is the restriction of $\Theta_{S(G)}^*$ to $S(G')$.

Consider an edge $e = \{x, y\}$ of the triangle of $G$ that contains $v$. Note that the facial triangles $C, C'$ containing $e$ have an isometric union, so by Lemma 3.4 we have $\{\overline{x}, xy\} \Theta_{S(G)}^* \{xy, \overline{y}\}$, which corresponds to our claim, since neither $x$ or $y$ can be of degree 3. If one of them—say $x$—was of degree 3 in $G'$, then now only the class $\gamma_x$ and $\gamma$ where merged. Since $G' \neq K_4$, not both $x$ and $y$ are of degree 3. Note furthermore that by Lemma 3.4 the edges incident to $v$ will all be in the class $\gamma$.

Finally, all the edges of the form $f = \{\overline{x}, vx\}$ are in relation $\Theta$ with each other. In order to see that they are the only constituents of the class $\gamma_v$ it suffices to notice that $d(\overline{x}, v) = d(x, v) + 1$ for all $v \in S(G')$. The result then follows by Lemma 2.2 (i).

5 $\Theta^*$ in subdivisions of chordal graphs

Recall that a graph is chordal if all its induced cycles are of length 3. As in fullerenes we define relation $\Phi$ on the edges of $S(G)$, by $e \Phi f$ if $e, f$ are opposite edges of a $C_6$.

Lemma 5.1 If $G$ is a chordal graph, then $\Phi_{S(G)}^* = \Theta_{S(G)}^*$.

Proof. Let $e \Theta_{S(G)} f$, where $e$ and $f$ are edges created by subdividing $\{a, b\}, \{c, d\} \in E(G)$, respectively. Then by Lemma 3.1 we have $\{a, b\} \Theta \{c, d\}$. Similarly as in the proof of Lemma 3.3, we have (up to symmetry) two options.

Case 1. $d_G(a, c) = d_G(b, d) = k$.

We can assume that $d_G(a, d) \in \{k, k + 1\}$ and $d_G(b, c) = k + 1$. Let $P = p_0 p_1 \ldots p_k$ and $P' = p'_0 p'_1 \ldots p'_k$ be shortest $a, c$- and $b, d$-paths, respectively. Clearly, $P$ and $P'$ must be disjoint since otherwise it cannot hold $d_G(a, d) \in \{k, k + 1\}, d_G(b, c) = k + 1$. The cycle $C$ formed by $\{a, b\}, P', \{d, c\}, P$ must have a chord. Inductively adding chords we can show that there is a chord of $C$ incident with $a$ or $b$. Since $P$ and $P'$ are shortest paths and the assumptions on distances hold, it follows that the latter chord must be incident with $a$ and the vertex $p'_1$ of $P'$. In particular, $d_G(a, d) = k$. Similarly, one can show that there must be a chord between $p'_1$ and $p_1$, and inductively between every $p_i p'_{i+1}$ for $0 \leq i < k$ and every $p_{i+1} p'_{i+1}$ for $0 \leq i < k - 1$. 


By the assumption on the distances, the only pair of subdivided edges of \{a, b\}, \{c, d\}, that is in relation \(\Theta_{S(G)}\), is \(\{b, \overline{ba}\} \Theta_{S(G)} \{\tau, \overline{cd}\}\), i.e., \(e = \{b, \overline{ba}\}\) and \(f = \{\tau, \overline{cd}\}\). Then
\[
\{b, \overline{ba}\} \Phi_{S(G)} \{\overline{ba}, \overline{ap_1}\} \Phi_{S(G)} \{\overline{p_1p_1'}, \overline{p_1p_1'}\} \Phi_{S(G)} \cdots \Phi_{S(G)} \{\overline{\tau, \overline{cd}}\}
\]

Case 2. \(d_G(a, c) = k, d_G(b, d) = k + 1\).

Then we have \(d_G(a, d) = d_G(b, c) = k + 1\). Similarly as above, shortest \(a, c\)- and \(b, d\)-paths, say \(P = p_0p_1 \ldots p_k\) and \(P' = p_0'p_1' \ldots p_k'\), cannot intersect. Using the same notation as above, \(C\) must have a chord incident with \(a\) or \(b\). By similar arguments, there must be a chord between every \(p_ip_{i+1}'\) and \(p_{i+1}'p_{i+1}\) for \(0 \leq i < k\).

By the assumption on the distances, the only pair of subdivided edges of \{a, b\}, \{c, d\}, that is in relation \(\Theta_{S(G)}\), is \(\{b, \overline{ba}\} \Theta_{S(G)} \{\overline{d, dc}\}\), i.e., \(e = \{b, \overline{ba}\}\) and \(f = \{\overline{d, dc}\}\). Then
\[
\{b, \overline{ba}\} \Phi_{S(G)} \{\overline{ba}, \overline{ap_1}\} \Phi_{S(G)} \{\overline{p_1p_1'}, \overline{p_1p_1'}\} \Phi_{S(G)} \cdots \Phi_{S(G)} \{\overline{d, dc}\}
\]

We have proved that \(\Theta_{S(G)} \subset \Phi^*_{S(G)}\), thus \(\Theta^*_S(G) = \Phi^*_{S(G)}\).

An edge of a graph \(G\) is called exposed if it is properly contained in a single maximal complete subgraph of \(G\). This concept was recently introduced in [10], where it was proved that \(G\) is a connected chordal graph if and only if \(G\) can be obtained from a complete graph by a sequence of removal of exposed edges. Denote by \(G^{-ee}\) the graph obtained from \(G\) by removing all its exposed edges. We will denote by \(c(G^{-ee})\) the number of connected components of \(G^{-ee}\). The singletons of \(G^{-ee}\) include the simplicial vertices of \(G\), and if \(G\) is 2-connected, its simplicial vertices coincide with singletons of \(G^{-ee}\). It is easy to verify that if \(G\) is a chordal graph, then \(\Theta^*\) consists of a single class. However, on the full subdivision of a chordal graph \(\Theta^*\) has the following structure.

**Theorem 5.2** Let \(G\) be a 2-connected, chordal graph. Then the coloring, that for an edge \{a, b\} with a being in the \(i\)-th connected component of \(G^{-ee}\) colors edge \{\(\overline{ab}, b\)\} with color \(i\), corresponds to the \(\Theta^*_{S(G)}\)-partition. In particular, \(|\Theta^*_{S(G)}| = c(G^{-ee})\).

**Proof.** We first prove that the above coloring of edges is a coarsening of \(\Theta^*_{S(G)}\). Let \(a\) be a vertex of \(G\) and \(b, c\) its neighbors. Since \(G\) is 2-connected, there is a \(b, c\)-path \(P\) that avoids \(a\). Pick \(P\) such that it is shortest possible. Then since \(G\) is chordal, \(a\) is adjacent to every vertex on \(P\), otherwise there exists a shorter path. Denote \(P = p_0p_1 \ldots p_k\), where \(p_0 = b\) and \(p_k = c\). Then \(\{\overline{p_0a, p_1}\} \Theta_{S(G)} \{\overline{p_ka}, \overline{p_k+1}\}\), proving that \(\{\overline{ba}, \overline{b}\} \Theta^*_{S(G)} \{\overline{a, \tau}\}\).
Furthermore, if $ab$ is not an exposed edge in $G$, then $ab$ lies in two maximal cliques. In particular, it lies in two isometrically touching triangles. By Lemma 3.4, $\{ab, \overline{ab}\} \Theta^*_{S(G)} \{\overline{a}, \overline{ab}\}$. By transitivity, and the above two facts, all the edges $\{ab, \overline{ab}\}$, with $a$ being in the same connected component of $G^{-ee}$, are in relation $\Theta^*_{S(G)}$.

Finally, we prove that no other edge besides the asserted is in $\Theta^*_{S(G)}$. Assume otherwise, and let $\{\overline{a}, \overline{ab}\} \Theta^*_{S(G)} \{\overline{c}, cd\}$ be such that $b$ and $d$ do not lie in the same connected component of $G^{-ee}$. By Lemma 5.1, we can assume that $\{\overline{a}, \overline{ab}\} \Phi_{S(G)} \{\overline{c}, cd\}$. But then the edges lie on a 6-cycle, implying that $b = d$. This cannot be.

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References


