A BIRD'S EYE VIEW OF THE CUT METHOD AND A SURVEY OF ITS APPLICATIONS IN CHEMICAL GRAPH THEORY

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Abstract

A general description of the cut method is presented and an overview of its applications in chemical graph theory is given. Applications include the Wiener index, the Szeged index, the hyper-Wiener index, the PI index, the weighted Wiener index, Wiener-type indices, and classes of chemical graphs such as trees, benzenoid graphs and phenylenes. A computation of the Wiener index of an arbitrary connected graph using its canonical metric representation is described. Algorithmic issues are also briefly mentioned as well as are the recently introduced CI index and related polynomials.

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1 Introduction

Let us describe the *cut method* in the following general form. For a given (molecular) graph G,

1. partition the edge set of G into classes $F_1, \ldots, F_k$, call them *cuts*, such that each of the graphs $G - F_i$, $i = 1, \ldots, k$, consists of two (or more) connected components; and

2. use properties (of the components) of the graphs $G - F_i$ to derive a required property of G.

The cut method can hardly be studied in the above generality, instead we are interested in classes of (chemical) graphs that allow applicable partitions into cuts and in relevant properties. Often a property of G, that we are interested in, is some graph invariant, for instance the Wiener index. We could be interested to obtain expressions for such invariants for certain (chemically) important classes of graphs or to develop fast algorithms for computing them.

The cut method turned out to be especially useful when if comes to metric properties of graphs. The key idea how the graphs $G - F_i$ can be used to obtain such properties of G is to find an isometric embedding $f : G \to H$, where H is a properly selected target graph and to use the image $f(G)$ to obtain distance properties of G. The key subidea is then to select H to be a Cartesian product graph. We introduce and explain the concepts mentioned in this paragraph in Section 2.

The most prominent class of chemical graphs for which the cut method turned out to be extremely fruitful is the class of benzenoid graphs. In fact, the 1995 paper [40] and the elaboration of its method for the computation of the Wiener index of benzenoid graphs (and, more generally, of partial cubes) from [24] can be considered as the starting point (at least in this context) of the cut method. We explain the method and its consequences in Section 3.

A similar approach that works for the Wiener index can be applied to the Szeged index as well. This is presented in Section 4. We continue with a section on the hyper-Wiener index. Again, the cut method is applicable, however, in this case it is slightly more involved than the corresponding methods for the Wiener and the Szeged index because the computation of the hyper-Wiener index requires not only graph distance but also squares of graphs distances. When arbitrary powers of distances are summed up, one speaks of Wiener-type indices. The cut method is once again fruitful by providing recursive theorems between such indices, see

Section 6.

In the subsequent section we consider the recently studied PI index in which case the cut method is already inherent in the definition of the index. Then, in Section 8 we introduce the notion of the weighted Wiener index, give an application of it, and use it for the expression of the Wiener index of an arbitrary graph. This last result uses a deep theory of the so-called canonical metric representation of a graph. In the concluding section several other topics related to the cut method are briefly mentioned.

2 Preliminaries

Let $G = (V, E)$ be a connected graph and $u, v \in V$. Then the *distance* $d_G(u, v)$ between u and v is the number of edges on a shortest u, v-path. (Other graph distances exist, some of then also of interest in mathematical chemistry, but they will are not treated in this paper.)

The *Cartesian product* $G \,\square\, H$ of graphs G and H is probably the most important graph product and is defined in the following way:

- $V(G \,\square\, H) = V(G) \times V(H)$;
- $E(G \,\square\, H)$ consists of pairs $(g, h)(g', h')$ where either $g = g'$ and $hh' \in E(H)$, or $gg' \in E(G)$ and $h = h'$.

The graphs G and H are called the *factors* of $G \,\square\, H$. The Cartesian product is commutative and associative. The latter property implies that products of several factors are well-defined. The fundamental metric property of the Cartesian product is that the distance function is additive:

$$d_{G \,\square\, H}((g, h), (g', h')) = d_G(g, g') + d_H(h, h')\,.$$

This property has been independently discovered several times, see for instance [51]. For more in-depth information on the Cartesian product operation see the book [28].

The simplest (yet challenging in many ways) Cartesian products are products in which all factors are the complete graph on two vertices K_2. These graphs are known as *hypercubes*. More precisely, the *n-cube* Q_n is the Cartesian product of n factors K_2, that is, $Q_n = \square_{i=1}^{n} K_2$. It is important to observe that the n-cube Q_n can be equivalently described as the graph whose vertex set consists of all n-tuples $b_1 b_2 \dots b_n$ with $b_i \in \{0, 1\}$, where two vertices are adjacent if the corresponding tuples differ in precisely one position.

A subgraph H of a graph G is *isometric* if for any vertices u and v of H,

$$d_H(u,v) = d_G(u,v)\,.$$

The class of graphs that consists of all isometric subgraphs of hypercubes turns out to be very important and has got the name *partial cubes.* We point out that (of course) hypercubes, even cycles, trees, median graphs (in particular acyclic cubical complexes), benzenoid graphs, phenylenes, and Cartesian products of partial cubes are all partial cubes.

Finally, in Fig. 1 the first three graphs from the circumcoronene series, H_k, $k \geq 1$, are shown.

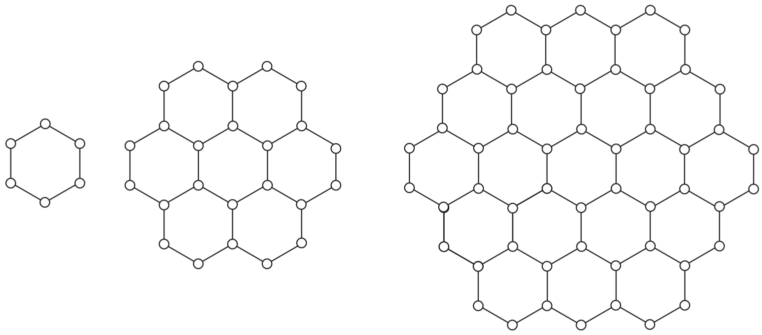

Figure 1: The first three graphs, H_1 H_2, and H_3, from the circumcoronene series

3 Wiener index

Recall that the *Wiener index* $W(G)$ of a graph $G = (V,E)$ is defined with

$$W(G) = \frac{1}{2}\sum_{u\in V}\sum_{v\in V} d_G(u,v)\,.$$

As we have already mentioned, the cut method was first implemented for a calculation of the Wiener index of benzenoid graphs. In fact, the method works for any partial cube as the next theorem asserts. For its formulation we need the following concepts.

Let G be a connected graph. Then $e = xy$ and $f = uv$ are in the *Djoković-Winkler relation* Θ [13, 50] if

$$d_G(x,u) + d_G(y,v) \neq d_G(x,v) + d_G(y,u)\,.$$

The relation Θ is always reflexive and symmetric, and is transitive on partial cubes. Therefore, Θ partitions the edge set of a partial cube G into equivalence classes, called Θ-*classes.* Now:

Theorem 3.1 ([40]) *Let G be a partial cube and let $F_1, \ldots, F_k$ be its Θ-classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G - F_i$. Then*

$$W(G) = \sum_{i=1}^{k} n_1(F_i) \cdot n_2(F_i)\,.$$

The proof of this theorem is short and typical for the cut method, hence it is worth to reproduce it here. So let G be a partial cube isometrically embedded into Q_k. (Note that the number of Θ-classes is equal to the dimension of the hypercube into G is embedded.) Then a vertex u of G can be considered as a binary k-tuple $u = u_1 u_2 \ldots u_k$, and the distance between two vertices is the number of positions in which they differ. For $b, b' \in \{0, 1\}$, let $\delta(b, b') = 0$ if $b = b'$, and $\delta(b, b') = 1$ if $b \neq b'$. Having this in mind we can compute as follows:

$$\begin{aligned}
W(G) &= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_G(u, v) \\
&= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_{Q_k}(u, v) \\
&= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} \sum_{i=1}^{k} \delta(u_i, v_i) \\
&= \sum_{i=1}^{k} \left(\frac{1}{2} \sum_{u \in V} \sum_{v \in V} \delta(u_i, v_i) \right) \\
&= \sum_{i=1}^{k} n_1(F_i) \cdot n_2(F_i)\,.
\end{aligned}$$

In benzenoid graphs the Θ-classes are precisely their orthogonal cuts. Hence if $\mathcal{C}$ is the set of orthogonal cuts of a benzenoid graph B, and for $C \in \mathcal{C}$ we let $n_1(C)$ and $n_2(C)$ be the number of vertices in the two components of $G - C$, respectively, then Theorem 3.1 specializes as follows [40, 24]:

$$W(B) = \sum_{C \in \mathcal{C}} n_1(C) \cdot n_2(C)\,. \tag{1}$$

We illustrate the use of (1) on the coronene H_2, see Fig. 2.

The coronene H_2 has three horizontal cuts, two of them being symmetric. Each of the these two cuts contributes $5 \cdot 19$ to $W(H_2)$, while contribution of the remaining cut is $12 \cdot 12$. Hence horizontal cuts contribute $2 \cdot 5 \cdot 19 + 12 \cdot 12 = 334$. Clearly, there are two more such groups of cuts, hence we conclude that $W(H_2) = 3 \cdot 334 = 1002$.

The above example demonstrates that the cut method (1) is very simple to apply and hence it is not surprising that it turned out to be extremely useful for obtaining closed expressions

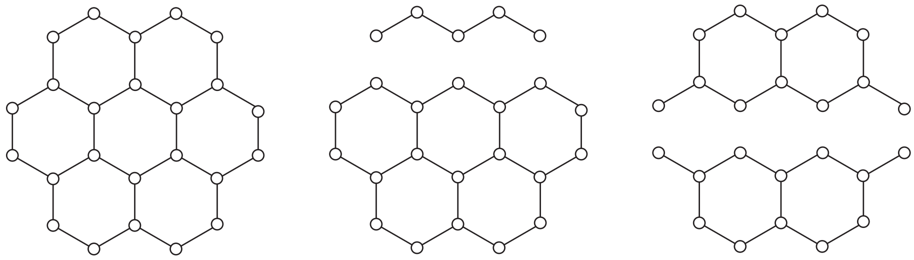

Figure 2: Coronene H_2 and two of its cuts

for the Wiener index of families of benzenoid graphs as was demonstrated in [22, 41]. The cut method was further applied in [16, 17] to obtain rules for the comparison of the Wiener index of various benzenoid isomers. For another aspect and application of Theorem 3.1 see [27].

A particular application of (1) is a straightforward, short proof of the following theorem that was obtained independently by two groups of authors.

Theorem 3.2 ([24, 48]) *For the graphs from the circumcoronene series, H_k, $k \geq 1$,*

$$W(H_k) = \frac{1}{5}\left(164k^5 - 30k^3 + k\right) .$$

Before Theorem 3.2 was proved, it was an open problem to obtain a closed formula for $W(H_k)$. The cut method turned the problem into a straightforward computation, as the above computation for $W(H_2)$ indicates.

In [20] Gutman and Cyvin demonstrated that several other non-distance properties of a benzenoid graph can be deduced from its cuts. The properties include the number of vertices of degree two and the number of internal vertices. Moreover, they also studied the so-called edge-cut sequences that are defined as the vectors whose components are the numbers of edges in cuts. Their main result asserts that any partition of the number $5h+1$ into $2h+1$ parts, each summand being an integer at least 2, yields an edge-cut sequence of some benzenoid graph. We note that the edge-cut sequences were recently studied for all partial cubes in [42]. In this case the vector corresponding to a partial cube contains the number of edges in its Θ-classes.

We conclude this section by pointing out that Chepoi, Deza and Grishukhin [6] extended Theorem 3.1 from partial cubes to the class of all L_1-graphs that contains also many (chemical) non-bipartite graphs. Here, a graph G is an L_1-*graph* if it admits a scale embedding into a hypercube, where a *scale embedding* of H into G is a mapping $\beta : V(H) \to V(G)$ such that

$d_G(\beta(u), \beta(v)) = \lambda d_H(u, v)$ holds for some fixed integer λ and all vertices $u, v \in V(H)$. Hence a scale embedding with $\lambda = 1$ is an isometric embedding.

4 Szeged index

The Szeged index was introduced in [31] in the following way. For an edge $e = uv$ of a connected graph G let $W_{uv} = \{x \in V(G) \mid d_G(x, u) < d_G(x, v)\}$. The set W_{vu} is defined analogously. Then the *Szeged index* of G is defined as:

$$Sz(G) = \sum_{uv \in E(G)} |W_{uv}| \cdot |W_{vu}| \,.$$

Now, let uv be an edge of a partial cube G and suppose that it belongs to the Θ-class F. Then it follows easily from definitions that W_{uv} and W_{vu} induce the connected components of $G - F$. Therefore, Theorem 3.1 has its variant for the Szeged index:

Theorem 4.1 *Let G be a partial cube and let $F_1, \ldots, F_k$ be its Θ-classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G - F_i$. Then*

$$Sz(G) = \sum_{i=1}^{k} |F_i| \cdot n_1(F_i) \cdot n_2(F_i) \,.$$

Theorem 4.1 was elaborated in [23] for benzenoid graphs. Since the Θ-classes of a benzenoid graph are its cuts, the result specializes to:

Corollary 4.2 ([23]) *Let B be a benzenoid graph and $\mathcal{C}$ the set of its orthogonal cuts. For $C \in \mathcal{C}$ let $n_1(C)$ and $n_2(C)$ be the number of vertices in the two components of $G - C$, respectively. Then*

$$Sz(B) = \sum_{C \in \mathcal{C}} |C| \cdot n_1(C) \cdot n_2(C) \,.$$

Consider again the coronene H_2 from Fig. 2. The computation of $Sz(H_2)$ goes along the same lines as the computation of $W(H_2)$, except that now we need to multiply each contribution with the size of the corresponding cut. Therefore,

$$Sz(H_2) = 3 \cdot \big(3 \cdot 2 \cdot 5 \cdot 19 + 4 \cdot 12 \cdot 12\big) = 3438 \,.$$

The cut method was then used on several classes of benzenoid graphs, in particular on the challenging circumcoronene series.

Theorem 4.3 ([23]) *For the graphs from the circumcoronene series, H_k, $k \geq 1$,*

$$Sz(H_k) = \frac{3}{2}k^2\left(36k^4 - k^2 + 1\right).$$

5 Hyper-Wiener index

The hyper-Wiener index WW was proposed by Randić in [47]. His definition was originally given only for trees and was extended to all connected graphs $G = (V, E)$ by Klein, Lukovits and Gutman [44] as follows:

$$WW(G) = \frac{1}{4}\sum_{u\in V}\sum_{v\in V} d_G(u,v) + \frac{1}{4}\sum_{u\in V}\sum_{v\in V} d_G(u,v)^2\,. \tag{2}$$

Note that the first term is one half of the Wiener index, while in the second we need to compute the squares of distances. The cut method is applicable also in this case, but because squares of distances are involved, the method, that we describe next, becomes slightly more involved.

Let G be a partial cube and let $F_1, \ldots, F_k$ be its Θ-classes. For each Θ-class F_i let u_iv_i be a representative of F_i. Then for any $1 \leq i < q$ let

$$n_{11}(F_i, F_j) = |W_{u_iv_i} \cap W_{u_jv_j}|\,, \quad n_{22}(F_i, F_j) = |W_{v_iu_i} \cap W_{v_ju_j}|\,,$$

and

$$n_{12}(F_i, F_j) = |W_{u_iv_i} \cap W_{v_ju_j}|\,, \quad n_{21}(F_i, F_j) = |W_{v_iu_i} \cap W_{u_jv_j}|\,.$$

Now we have the following theorem.

Theorem 5.1 ([34]) *Let G be a partial cube with Θ-classes $F_1, \ldots, F_k$ and representatives $u_iv_i \in F_i$, $1 \leq i \leq k$. Then*

$$WW(G) = W(G) + \sum_{i=1}^{k}\sum_{j=i+1}^{k}\Big(n_{11}(F_i,F_j)\cdot n_{22}(F_i,F_j) + n_{12}(F_i,F_j)\cdot n_{21}(F_i,F_j)\Big)\,. \tag{3}$$

The key step in proving Theorem 5.1 is to show that

$$\sum_{u\in V}\sum_{v\in V} d_G(u,v)^2 = 2W(G) + 4\sum_{i=1}^{k}\sum_{j=i+1}^{k}\Big(n_{11}(F_i,F_j)\cdot n_{22}(F_i,F_j) + n_{12}(F_i,F_j)\cdot n_{21}(F_i,F_j)\Big)\,.$$

The result then follows immediately by plugging the last equality into (2).

Theorem 5.1 was also derived in [39] as a consequence of the main theorem.

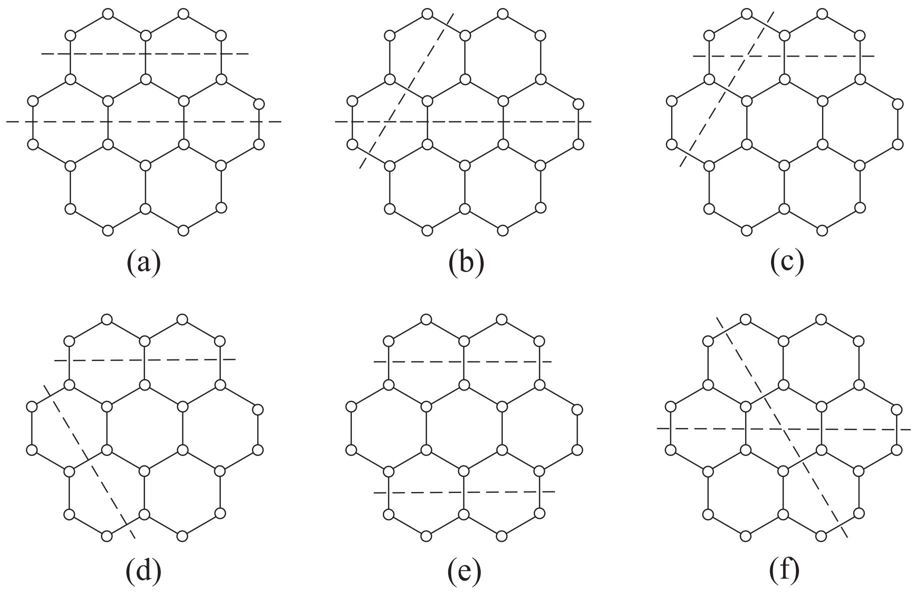

Figure 3: Types of pairs of cuts in the coronene

For an example consider again the coronene. It contains 9 cuts, hence there are $\binom{9}{2} = 36$ pairs of cuts to be considered. These cuts can be grouped into 6 types that are shown in Fig. 3.

There are 6, 12, 6, 6, 3, and 3 pairs of cuts in the cases (a), (b), (c), (d), (e), and (f), respectively. Hence the second term of Theorem 5.1 gives

$$6(5\cdot 12+0\cdot 7)+12(4\cdot 11+1\cdot 8)+6(2\cdot 16+3\cdot 3)+6(5\cdot 5+0\cdot 14)+3(5\cdot 5+0\cdot 14)+3(4\cdot 4+8\cdot 8) = 1695\,.$$

Since $W(H_2) = 1002$ we conclude by Theorem 5.1 that $WW(H_2) = 2697$.

We have already mentioned that a closed expression for the Wiener index of the circumcoronene series was quite a challenge. Hence an even more challenging task was to obtain an expression for the hyper-Wiener index of this class of chemical graphs. The cut method is applicable also this case, but the computations are not so short any more—the majority of the paper [52] consists of the computation for the following result.

Theorem 5.2 ([52]) *For the graphs from the circumcoronene series, H_k, $k \geq 1$,*

$$WW(H_k) = \frac{548}{15}k^6 + \frac{82}{5}k^5 - \frac{55}{6}k^4 - 3k^3 + \frac{17}{15}k^2 + \frac{1}{10}k\,.$$

For further information on the cut method applied on the hyper-Wiener index see [43].

6 Wiener-type indices

Let λ be an arbitrary real (or complex) number. Then the Wiener index can be widely generalized by the following definition proposed by Gutman in [18]:

$$W_\lambda(G) = \sum_{u,v} d_G(u,v)^\lambda \,.$$

Of course, $W_1(G) = W(G)$, but this definition covers several additional previously studied topological indices, for instance W_{-2}, W_{-1}, and $W_{-1/2}$, cf. [12]. Note also that $WW(G) = \frac{1}{2}W_1(G) + \frac{1}{2}W_2(G)$.

Using the cut method the following theorem can be proved.

Theorem 6.1 ([38]) *Let B be a benzenoid graph and $\mathcal{C}$ the set of its orthogonal cuts. Then*

$$W_{\lambda+1}(B) = |\mathcal{C}|\, W_\lambda(B) - \sum_{C\in\mathcal{C}} W_\lambda(B - C) \,.$$

Using Theorem 6.1, the following relation between the hyper-Wiener index and the Wiener index of a benzenoid graph (and again, of an arbitrary partial cube) can be deduced.

Corollary 6.2 ([38]) *Let B be a benzenoid graph and $\mathcal{C}$ the set of its orthogonal cuts. Then*

$$WW(B) = \frac{|\mathcal{C}|+1}{2} W(B) - \frac{1}{2} \sum_{C\in\mathcal{C}} W(B-C) \,.$$

In fact, Theorem 6.1 and Corollary 6.2 hold for arbitrary partial cubes. See [39] for the proof (using the cut method, of course) as well as for additional applications of Theorem 6.1.

7 PI index

The PI index is a recently introduced index [33] that received a considerable attention, see for instance [3, 8, 32]. For an edge $e = uv$ of a connected graph G let $m_u(e|G)$ be the number of edges of G whose distance to u is smaller than the distance to v; define $m_v(e|G)$ analogously. Then the *PI index* of G is:

$$PI(G) = \sum_{e=uv\in E(G)} \Big(m_u(e|G) + m_v(e|G) \Big) \,.$$

(See [2] for three different variations of this concept.)

Recall that for an edge $e = uv$ of a connected graph G we denote with W_{uv} the set of vertices of G that are closer to u than to v. By abuse of language we also identify W_{uv} with the subgraph of G induced by the vertices from W_{uv}. Suppose now that uv is an edge of a bipartite graph G and x a vertex of G. Then $d(x,u) = d(x,v)$ would yield an odd cycle in G. Therefore, an edge that is closer to u than to v lies in W_{uv} and an edge that is closer to v than to u lies in W_{vu}. Consequently, if G is a bipartite graph, then its PI index can be equivalently expressed as

$$PI(G) = \sum_{uv \in E(G)} \Big(|E(W_{uv})| + |E(W_{vu})| \Big) \,.$$

Let G be a partial cube and uv and xy edges from the same Θ-class. Then it easily follows from definitions (and is also well-known) that the notation can be selected such that $W_{uv} = W_{xy}$ and $W_{vu} = W_{yx}$. Hence the contribution of any edge from a given Θ-class to $PI(G)$ is the same. Therefore, the cut method is applicable by partitioning $E(G)$ into Θ-classes. As we have pointed out earlier, in the case of benzenoid graphs the Θ-classes are their orthogonal cuts. This is precisely the idea followed by John, Khadikar and Singh in [29]. But the cut method works much more generally as shown in [36]. This general cut method for the PI index goes as follows.

For a graph G, a partition $E_1, \ldots, E_k$ of $E(G)$ is a *PI-partition* if for any i, $1 \le i \le k$, and for any $uv, xy \in E_i$ we have $W_{uv} = W_{xy}$ and $W_{vu} = W_{yx}$. Let also ${}_uW_v$ be the set of all vertices that are at equal distance from u and v and for $X \subseteq V(G)$ let ∂X denote the set of edges of G with one end vertex in X and the other not in X. Then we have:

Theorem 7.1 ([36]) *Let $E_1, \ldots, E_k$ be a PI-partition of a graph G and let $u_iv_i \in E_i$, $1 \le 1 \le k$, be representatives of E_i's. Then*

$$PI(G) = |E(G)|^2 - \sum_{i=1}^{k} |E_i| \cdot \Big(|E_i| + |E({}_{u_i}W_{v_i})| + |\partial\, {}_{u_i}W_{v_i}| \Big) \,.$$

If G is bipartite then ${}_{u_i}W_{v_i} = \emptyset$ and therefore $\partial\, {}_{u_i}W_{v_i} = \emptyset$. Thus:

Corollary 7.2 ([36]) *Let G be a bipartite graph. Then using the notation of Theorem 7.1,*

$$PI(G) = |E(G)|^2 - \sum_{i=1}^{k} |E_i|^2 \,.$$

8 Weighted Wiener index and canonical metric representation

In this section we give a general theorem proved in [35] for the Wiener index of an arbitrary connected graph. In this way Theorem 3.1 becomes a very special case.

In order to give an appealing formulation of the announced theorem, the concept of the weighted Wiener index is useful. A *weighted graph* (G, w) is a graph G together with a *weight function* $w : V(G) \to \mathbb{R}$. *The Wiener index* $W(G, w)$ *of a weighted graph* (G, w) is defined as [37]:

$$W(G,w) = \frac{1}{2} \sum_{u \in V} \sum_{v \in V} \; w(u) \; w(v) \; d_G(u,v) \, .$$

Clearly, if all the weights are 1 then $W(G, w) = W(G)$.

Another concept that we need for the main theorem is the canonical metric representation of a graph due to Graham and Winkler [15].

Recall that the relation Θ is always reflexive and symmetric. Let Θ^* be the transitive closure of Θ. Then Θ^* is an equivalence relation on $E(G)$ for any connected graph and it partitions the edge set of G into Θ^*-*classes*. For computing Θ^*-classes it is useful to know the following basic facts. Since two adjacent edges of G are in relation Θ if and only if they belong to a common triangle, all the edges of a given complete subgraph of G will be in the same Θ^*-class. Also, since an edge e of an isometric cycle C of G is in relation Θ with its antipodal edge(s) on C, all the edges of an odd cycle will be in the same Θ^*-class.

The *canonical metric representation* α of a connected graph G is defined as follows.

- Let G be a connected graph and $F_1, \ldots, F_k$ its Θ^*-classes.
- Define *quotient graphs* G/F_i, $i = 1, \ldots, k$, as follows. Its vertices are the connected components of $G - F_i$, two vertices C and C' being adjacent if there exist vertices $x \in C$ and $y \in C'$ such that $xy \in F_i$.
- Define $\alpha : G \to \Box_{i=1}^{k} G/F_i$ with

  $$\alpha : u \mapsto (\alpha_1(u), \ldots, \alpha_k(u)) \, ,$$

  where $\alpha_i(u)$ is the connected component of $G - F_i$ that contains u.

The fundamental property of α is that $\alpha(G)$ is an isometric subgraph of $\Box_{i=1}^{k} G/F_i$ [15], but it has other interesting properties. For instance, it is irredundant, has the largest possible number of factors among all irredundant isometric embeddings and is unique among such embeddings. See [9, 28] for more information on this embedding as well as for proofs.

Let G be an arbitrary connected graphs and

$$\alpha : G \to \Box_{i=1}^{k} G/F_i$$

the canonical metric representation of G. Let $(G/F_i, w_i)$ be "natural" weighted graphs: the weight of a vertex of G/F_i is the number of vertices in the corresponding connected component of $G - F_i$. Then:

Theorem 8.1 ([35]) *For any connected graph G,*

$$W(G) = \sum_{i=1}^{k} W(G/F_i, w_i)\,.$$

Note that Theorem 8.1 is also a particular instance of the cut method: in this case the cuts are the Θ^*-classes, and we derive the Wiener index of G from the connected components of the graphs $G - F_i$ via the weighted Wiener index.

For a small example illustrating Theorem 8.1 consider the fullerene $C_{20}(2)$ from Fig. 4.

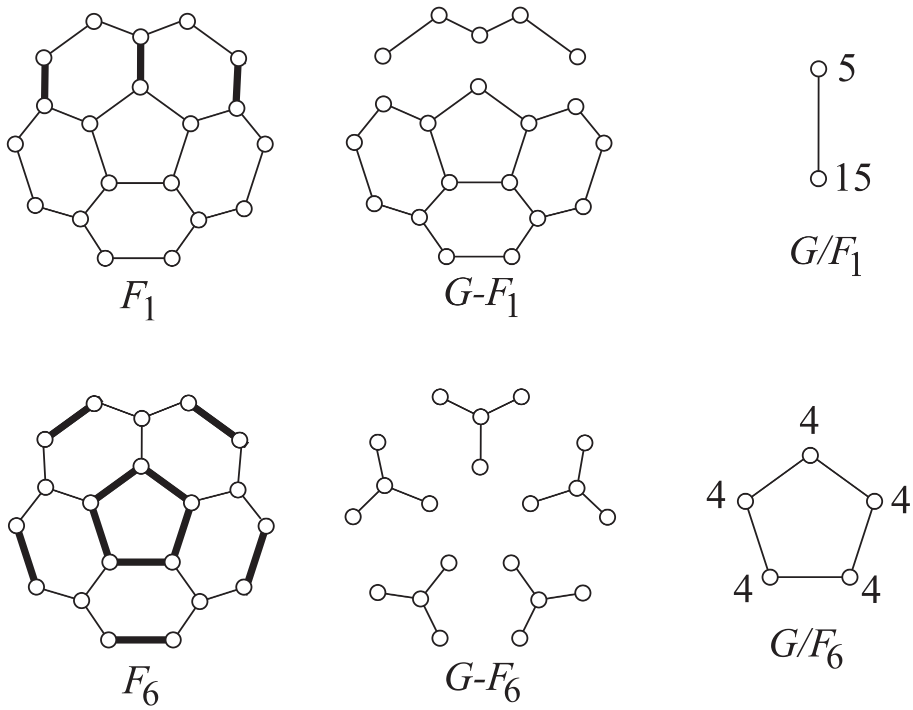

Figure 4: Computing the Wiener index of $C_{20}(2)$

$C_{20}(2)$ has 6 Θ^*-classes $F_1, \ldots, F_6$. The class F_1 is shown in the top left part of the figure. Classes $F_2, \ldots, F_5$ are symmetric and hence not drawn. The last class F_6 is given on the bottom left. Then the graphs obtained be removing F_1 and F_6, and the quotient graphs G/F_1 and G/F_6 together with the corresponding weight functions w_1 and w_6 are shown. Now, $W(G/F_i, w_i) = 5 \cdot 15 = 75$, $i = 1, \ldots, 5$ and $W(G/F_6, w_6) = 5 \cdot 4 \cdot 4 + 5 \cdot 2 \cdot 4 \cdot 4 = 240$. Therefore, $W(C_{20}(2)) = 5 \cdot 75 + 240 = 615$, see also [1].

9 Concluding remarks

In this section we briefly present additional applications of the cut method.

9.1 Fast algorithms

The cut method is also useful for developing fast algorithms for computing distance-based graph invariants. A detailed overview of the related approached was given earlier in [14, Section 3], hence here we will only briefly mention this point of view of the cut method.

Suppose B is a benzenoid graph. Then the edge set of B can be partitioned into three cuts as follows: each cut consists of all parallel edges. Then, making quotient graphs just as it is done in the canonical metric representation, we obtain three trees T_1, T_2, T_3. The key observation of Chepoi [5] is that B embeds isometrically into $T_1 \,\square\, T_2 \,\square\, T_3$. Now, defining the weights on these trees in the analogous way as it is done for the canonical representation, we get the following result.

Theorem 9.1 ([7]) *Let B be a benzenoid graph and let (T_1, w_1), (T_2, w_2), and (T_3, w_3) be the corresponding weighted trees. Then*

$$W(B) = W(T_1, w_1) + W(T_2, w_2) + W(T_3, w_3)\,.$$

The Wiener index of a tree can be computed in linear time [45] as well as it can be the weighted Wiener index [7]. Therefore Theorem 9.1 leads to a linear algorithm for computing the Wiener index of a benzenoid graph.

A similar approach works for the Szeged index as well [7]. That is, Theorem 9.1 also leads to a linear algorithm for computing the Szeged index of a benzenoid graph.

9.2 Phenylenes

Phenylenes are a class of chemical compounds in which the carbon atoms form 6-cycles and 4-cycles, where each 4-cycle is adjacent to two disjoint 6-cycles, and no two 6-cycles are adjacent. The respective graphs are also called *phenylenes*.

Given a phenylene PH, its hexagonal squeeze HS is the graph obtained from PH by identifying for each 4-cycle C the two edges of C that lie in the neighboring 6-cycles. Let (HS, w) be the weighted hexagonal squeeze, where the weight of the vertices that were identified is 2, while the weights of the remaining vertices are 1. The inner dual ID of PH is the graph with vertices corresponding to the 6-cycles and 4-cycles of PH, two vertices being adjacent if the corresponding cycles share an edge. Then using the cut method we can prove:

Theorem 9.2 ([37]) *For a phenylene PH,*

$$W(PH) = W(HS, w) + 36\, W(ID)\,.$$

For similar relations between the Wiener index of phenylenes and their hexagonal squeezes see [25, 26, 46].

Very recently Gutman and Ashrafi [19] applied the cut method on the phenylenes for the PI index and obtained the following nice result.

Theorem 9.3 *For a phenylene PH with h hexagons,*

$$PI(PH) = 4\, PI(HS) - 36\, h^2 - 44\, h + 8\,.$$

9.3 Quasi-orthogonal cuts, CI index, and related polynomials

Suppose G is a plane bipartite graph with isometric faces. A *quasi-orthogonal cut* with respect to a given edge is the smallest subset of edges closed under taking opposite edges on faces. Recalling that an edge f of an isometric face F is in relation Θ to its antipodal edge f' on F we observe that on partial cubes quasi-orthogonal cuts coincide with the Θ-classes. However, if Θ is not transitive, quasi-orthogonal cuts present a new concept applicable for the cut method.

Based on quasi-orthogonal cuts several new concepts have been recently introduced into mathematical chemistry. First, the CI index [30] of a graph G is defined with

$$CI(G) = |E(G)|^2 - \sum_{i=1}^{k} |E_i|^2\,,$$

where $E_1, \ldots, E_k$ are the quasi-orthogonal cuts of G. (Note the close similarity of the definition of the CI index with Corollary 7.2.) Second, three counting polynomials, the Omega polynomial, the Theta polynomial and the PI polynomial, all of them defined via quasi-orthogonal cuts, were introduced in [4, 10]. See also [11] for the mutual inter-relations between these polynomials.

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