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On the Wiener Index of Fibonacenes *

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Abstract

The Wiener index is a distance-based topological index defined as the sum of distances between all pairs of vertices in a graph. Fibonacenes are a class of unbranched catacondensed benzenoid hydrocarbons having zig-zag structure. We deal mainly with so-called collective properties of the Wiener index, i. e. the main results don't reflect the property of Wiener index of any particular fibonacene, but a collective property of sets of such graphs. In particular, some results on degeneracy classes of the Wiener index of fibonacenes are presented.

1. Introduction

In this paper we are concerned with finite undirected connected graphs. The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. If u and v are vertices of G, then the number of edges in the shortest path connecting them is said to be their distance and is denoted by $d(u,v)$.

The Wiener index is a well-known distance-based topological index introduced as structural descriptor for acyclic organic molecules [28]. It is defined as the sum of distances between all unordered pairs of vertices of a graph G:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

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The Wiener index is extensively used in theoretical chemistry for the design of quantitative structure–property relations (mainly with physico-chemical properties) and quantitative structure–activity relations including biological activities of the respective chemical compounds. Since benzenoid hydrocarbons are attracting the great interest of theoretical chemists, the theory of the Wiener index of the respective molecular graphs have been intensively developed in the last three decades. The bibliography on the Wiener index and its applications can be found in books [4, 12, 26, 27] and reviews [3, 9, 10, 22, 24]. In this paper we study the Wiener index for hexagonal chains having zig-zag structure.

2. Fibonacenes

A hexagonal system is a connected plane graph in which every inner face is bounded by hexagon. An inner face with its hexagonal bound is called a *hexagonal ring* (or simply *ring*). Two hexagonal rings are either disjoint or have exactly one common edge (adjacent rings), and no three rings share a common edge. A vertex of a hexagonal system belongs to at most three hexagonal rings. A hexagonal system is called *catacondensed* if it does not possess three hexagonal rings sharing a common vertex. A ring having exactly one adjacent ring is called *terminal*. A catacondensed hexagonal system having exactly two terminal rings is called a *hexagonal chain*. A ring adjacent to exactly two other rings has two vertices of degree 2. If these two vertices are adjacent, then the ring is angularly annelated, if these two vertices are not adjacent, then it is linearly annelated. A *fibonacene* is a hexagonal chain without linearly annelated hexagonal rings. Examples of fibonacenes are shown in Fig. 1. The name of these chains comes from the fact that the number of perfect matchings of any fibonacene relates with the Fibonacci numbers. Detailed information about properties of fibonacenes can be found in [1, 16, 17].

Throughout this article h always denotes the number of hexagonal rings. A molecular graph representing any fibonacene with h rings has $4h+2$ vertices and $5h+1$ edges. The edge set may be divided into three subsets with respect of degree of incident vertices: $h+4$ edges connect two vertices of degree two, $2h-3$ edges connect two vertices of degree 3, and $2h$ edges connect vertices of degree 2 and 3.

Denote by $\mathcal{F}_h$ and $\mathcal{S}_h$ the set of all fibonacenes and all symmetrical fibonacenes with

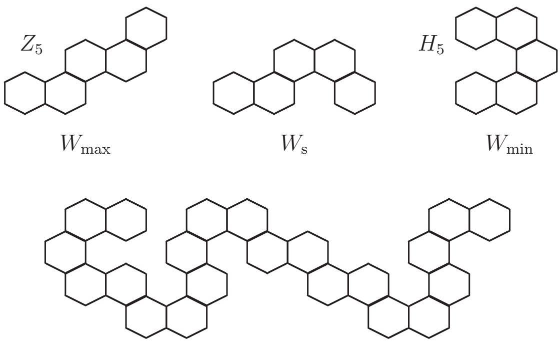

Figure 1. Fibonacenes with five rings and a large fibonacene.

h rings, respectively. The numbers of fibonacenes in these sets are [1]

$$|\mathcal{F}_h| = \begin{cases} 2^{h-4} + 2^{(h-5)/2}, & \text{if } h \text{ is odd} \\ 2^{h-4} + 2^{(h-4)/2}, & \text{if } h \text{ is even,} \end{cases}$$

$$|\mathcal{S}_h| = \begin{cases} 2^{(h-3)/2}, & \text{if } h \text{ is odd} \\ 2^{(h-2)/2}, & \text{if } h \text{ is even.} \end{cases}$$

Among the fibonacenes with a fixed number of rings two are extremal with regard to their Wiener indices: the helicene H_h and the zig-zag fibonacene Z_h (see examples in Fig. 1). If all hexagonal rings are regular, then the helicene has the spiral structure while all rings of the zig-zag fibonacene lie on a straight line. Their Wiener indices have the minimal and the maximal values, respectively [2, 13]:

$$W_{\text{min}} = W(H_h) = \frac{1}{3}\left(8h^3 + 72h^2 - 26h + 27\right),$$

$$W_{\text{max}} = W(Z_h) = \frac{1}{3}\left(16h^3 + 24h^2 + 62h - 21\right).$$

Denote by W_{s} the average value of W_{min} and W_{max}, i. e.

$$W_{\text{s}} = \frac{1}{2}\left(W_{\text{min}} + W_{\text{max}}\right) = 4h^3 + 16h^2 + 6h + 1.$$

Further, these three W-values will be considered only for graphs with h rings. The sum of values of the Wiener index for a subset of fibonacenes $\mathcal{G} \subseteq \mathcal{F}_h$ will be denoted by $W(\mathcal{G}) = \sum_{G \in \mathcal{G}} W(G)$. Denote by $Val(\mathcal{G})$ the set of W-values for fibonacenes of $\mathcal{G} \subseteq \mathcal{F}_h$, $Val(\mathcal{G}) = \{W(G) \,|\, G \in \mathcal{G}\}$.

3. Branching graph

The concept of branching graphs has been introduced for characterization the branchings in hexagonal systems [19]. The *branching graph*, $B(G)$, of a hexagonal system G is called a subgraph induced by all vertices of degree 3 in G. Since a fibonacene has no three linearly annelated hexagonal rings, its branching graph is an acyclic connected graph (*branching tree*). As an illustration, consider fibonacene G shown in Fig. 2a. Bold edges form its branching tree $B(G)$. Every vertex of a branching tree has degree 1, 2 or 3. The numbers of vertices and edges of $B(G)$ are $2h-2$ and $2h-3$, respectively.

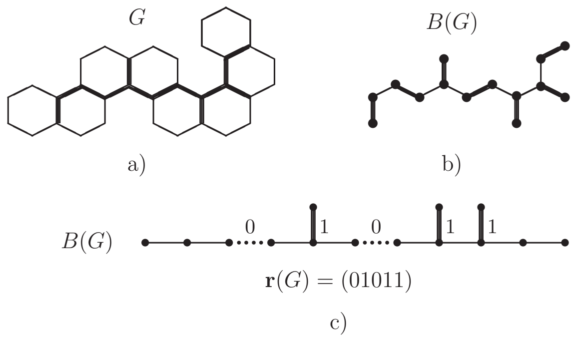

Figure 2. Branching tree $B(G)$ and a code $\mathbf{r}(G)$ for fibonacene $G \in \mathcal{F}_8$.

A fibonacene's edge is called *cut-edge* if it belongs to two rings (cut a paper model of a fibonacene along this edge produces two fibonacenes). Obviously, all cut-edges of a fibonacene belong to its branching tree (cut-edges are depicted by bold lines in Fig. 2b). Denote by $C(G)$ the set of all cut-edges of a fibonacene $G \in \mathcal{F}_h$ except cut-edges belonging to the first and the last hexagons. Then $|C(G)| = h-3$. Every cut-edge of $C(G)$ is adjacent with two non-cut-edges. The set $C(G)$ can be presented as disjoint union of two subsets, $C(G) = U(G) \cup Z(G)$, where an edge of $U(G)$ is incident with a vertex of degree 3 in $B(G)$ whereas the both end-vertices of an edge of $Z(G)$ have degree 2. For the branching tree $B(G)$ in Fig. 2c, three edges of $U(G)$ and two edges of $Z(G)$ are shown by bold and dotted lines, respectively. For example, $Z = \emptyset$ for the helicene and $U = \emptyset$ for the zig-zag fibonacene. Let $z = |Z(G)|$ and $u = |U(G)|$.

4. Representation of fibonacenes

Since fibonacenes have zig-zag structure, there is an obvious way to represent their structures as binary codes. We associate a binary code with the branching tree of a fibonacene $G \in \mathcal{F}_h$ as shown in Fig. 2c. Every cut-edge of $U(G)$ corresponds to 1 in the code while every cut-edge of $Z(G)$ corresponds to 0. The length of fibonacenes' codes is $h-3$. A fibonacene with non-trivial symmetry has symmetrical code. For instance, the helicene H_7 and the zig-zag fibonacene Z_7 have the following codes: (1111) and (0000). Two binary codes (11000) and (00011) induce the same fibonacene. Denote by $\mathbf{r}(G)$ a code corresponding to a fibonacene G. We will assume that $\mathbf{r}(G)$ is equal to one of possible codes of G. For further considerations, it is not important how to choose $\mathbf{r}(G)$. A fibonacene induced by a code $\mathbf{r}$ will be denoted by $G(\mathbf{r})$. Binary representation is useful for computer generation of fibonacenes.

5. Calculating formulas for the Wiener index

In this section, we derive two calculating formulas for the Wiener index based on cut-edges of fibonacenes. Denote by $V_3(G)$ the set of all vertices of degree 3 in a graph G. Let $W_{33}(G)$ be the sum of distances between vertices of degree 3 in G,

$$W_{33}(G) = \sum_{\{u,v\} \subseteq V_3(G)} d(u,v).$$

There is a simple relation between the quantity W_{33} and the Wiener index of catacondensed hexagonal systems [11].

Proposition 1. *For an arbitrary catacondensed hexagonal system G with h rings*,

$$W(G) = 4W_{33}(G) + 3(8h^2 + 2h - 1).$$

Since all shortest paths between vertices of degree 3 in a fibonacene $G \in \mathcal{F}_h$ form its branching tree $B(G)$, we can write

$$W(G) = 4W(B(G)) + 3(8h^2 + 2h - 1).$$

Every vertex v of degree 3 in a branching tree $B(G)$ has one neighbor u of degree 1. The structures of a fibonacene G and its branching tree $B(G)$ are shown in Fig. 3a. To calculate the Wiener index of a branching tree, it is convenient to apply the Doyle–Graver method [14]. Denote by n_1 and n_2 the number of vertices in two subtrees T_1 and T_2.

Proposition 2. *Let B be a branching tree with n vertices. Then*

$$W(B) = \binom{n+1}{3} - \sum_{v \in V_3(B)} n_1 n_2.$$

Consider an edge $e = (u,v) \in U(G)$ for $G \in \mathcal{F}_h$ shown in Fig. 3a. After cutting along this edge, one can obtain two fibonacenes with $h_1(e)$ and $h_2(e)$ rings, $h_1(e) + h_2(e) = h$. Then $n_1 = 2(h_1(e) - 1)$ and $n_2 = 2(h_2(e) - 1)$. Since there is a bijection between vertices of degree 3 and edges of $U(G)$, we can write that the sum of Doyle–Graver formula goes over all edges of $U(G)$. Applying Propositions 1 and 2, we have

$$W(G) = 4\binom{2h-1}{3} - 4\sum_{e \in U(G)} 2(h_1(e)-1) \cdot 2(h_2(e)-1) + 3(8h^2 + 2h - 1).$$

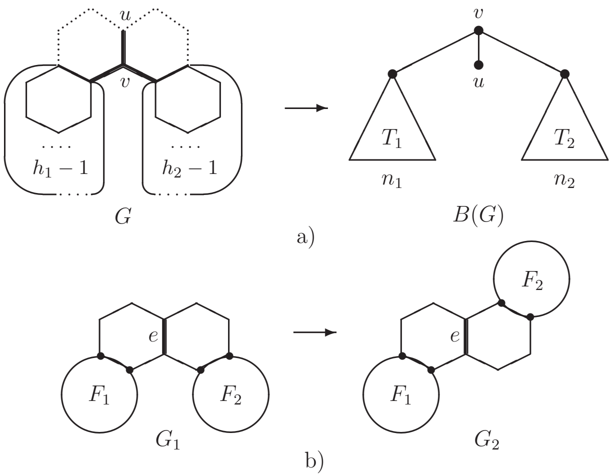

Figure 3. Calculating the Wiener index.

After simplification, one obtains the first formula:

$$W(G) = W_{\max} + 16\,u(h-1) - 16\sum_{e \in U(G)} h_1(e)h_2(e). \qquad (1)$$

To derive the second formula, we apply a method developed in [23]. Consider fibonacenes $G_1, G_2 \in \mathcal{F}_h$ and a graph transformation $G_1 \to G_2$ shown in Fig. 3b. Here F_1 and F_2 are arbitrary fibonacenes. This transformation consists of the rotation of the subgraph F_2 around the edge e, where $e \in U(G_1)$ and $e \in Z(G_2)$. Let $h_1(e) = h(F_1) + 1$ and

$h_2(e) = h(F_2)+1$. Then the Wiener indices of the graphs G_1 and G_2 satisfy the following equation [23]:

$$W(G_1) = W(G_2) - 16\,(h_1(e)-1)(h_2(e)-1).$$

It is easy to see that every fibonacene $G \in \mathcal{F}_h$ may be obtained from the helicene H_h by a sequence of such operations, so that every respective edge of H_h is used only once. All transformations are induced by the edge set $Z(G)$. By inverse operations, every fibonacene can be transformed to the helicene. Applying the above equality to all transformations, we get the second formula:

$$W(G) = W_{\min} - 16\,z(h-1) + 16 \sum_{e\in Z(G)} h_1(e)h_2(e). \tag{2}$$

The obtained formulas (1) and (2) are based on two sets of cut-edges of fibonacenes and have similar forms.

6. Linked fibonacenes

Let $G, G' \in \mathcal{F}_h$ and $C(G) = \{e_1, e_2, ..., e_{h-3}\}$, $C(G') = \{e'_1, e'_2, ..., e'_{h-3}\}$. Two fibonacenes G and G' are called *linked* if there are sequential numberings of their cut-edges such that $e_i \in U(G)$ and $e'_i \in Z(G')$ or $e_i \in Z(G)$ and $e'_i \in U(G')$ for every $i = 1, 2, ..., h-3$. In other words, two i-th cut-edges can not belong to the set $U(G)$ or $Z(G)$ simultaneously. Denote by $\overline{G}$ the linked graph for a fibonacene G. It is clear that $\overline{\overline{G}} = G$. If G_1 and G_2 are linked graphs then $\mathbf{r}(G_2)$ is the bitwise negation of $\mathbf{r}(G_1)$, i. e. $\mathbf{r}(G_2) = \overline{\mathbf{r}}(G_1)$. Examples of linked fibonacenes and their codes are shown in Fig. 4a.

Proposition 3. *For a fibonacene $G \in \mathcal{F}_h$,*

$$W(G) + W(\overline{G}) = W_{\min} + W_{\max} = 8h^3 + 32h^2 + 12h + 2.$$

Proof. Apply formula (1) to a fibonacene G and formula (2) to its linked graph $\overline{G}$. It is easy to see that $u(G) = z(\overline{G})$ and the sums of formulas (1) and (2) are also equal. □

A fibonacene G is called *self-linked* if $\overline{G} \cong G$ (see Fig. 4b). The set of self-linked fibonacenes with h hexagonal rings will be denoted by $\mathcal{L}_h$. If G is a self-linked fibonacene, then $|U(G)| = |Z(G)|$. It is clear that self-linked fibonacenes exist if the number of rings h is odd ($h-3$ is even). Any symmetrical fibonacene is non-self-linked. Since the first half of a self-linked fibonacene defines the second one, the number of self-linked fibonacenes

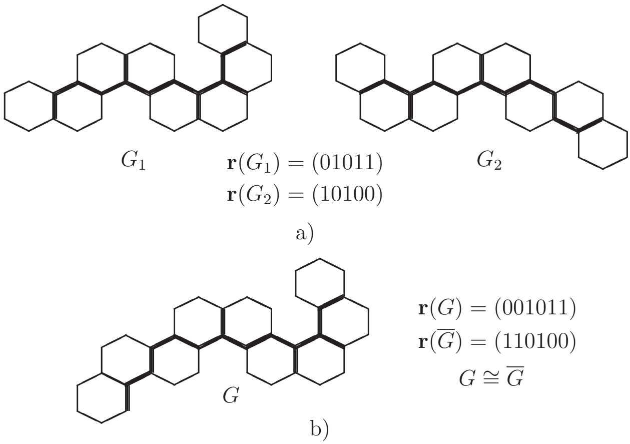

Figure 4. Linked and self-linked fibonacenes.

is $|\mathcal{L}_h| = 2^{(h-3)/2}/2 = 2^{(h-5)/2}$. The following result shows that the Wiener indices of all self-linked fibonacenes coincide.

Corollary 4. *For a self-linked fibonacene $G \in \mathcal{F}_h$,*

$$W(G) = 4h^3 + 16h^2 + 6h + 1 = W_s.$$

A set of fibonacenes $\mathcal{G}$ is called *complete* if for every fibonacene $G \in \mathcal{G}$ the set always contains its linked graph $\overline{G}$. If $\mathcal{G}_1$, $\mathcal{G}_2 \subseteq \mathcal{F}_h$ are arbitrary complete sets then $\mathcal{G}_1 \cup \mathcal{G}_2$, $\mathcal{G}_1 \cap \mathcal{G}_2$ and $\mathcal{G}_1 \setminus \mathcal{G}_2$ are also complete sets in $\mathcal{F}_h$. Cardinalities of a complete set and its subset of all self-linked graphs have the same parity.

Corollary 5. *For a complete set of fibonacenes $\mathcal{G} \subseteq \mathcal{F}_h$,*

$$W(\mathcal{G}) = \sum_{G \in \mathcal{G}} W(G) = W_s \cdot |\mathcal{G}|.$$

Proof. The proof follows from the equalities

$$\sum_{G \in \mathcal{G}} W(G) = \frac{1}{2}\left(\sum_{G \in \mathcal{G}} W(G) + \sum_{G \in \mathcal{G}} W(\overline{G})\right) = \sum_{G \in \mathcal{G}} \left(W(G) + W(\overline{G})\right)/2 = W_s \cdot |\mathcal{G}|. \ \square$$

It is clear that the sets of all symmetrical fibonacenes $\mathcal{S}_h$, all self-linked fibonacenes $\mathcal{L}_h$, and all fibonacenes $\mathcal{F}_h$ are complete.

Corollary 6. *For the average value W_{avr} of fibonacenes of $\mathcal{F}_h$,*

$$W_{\text{avr}} = \frac{W(\mathcal{F}_h)}{|\mathcal{F}_h|} = W_s = 4h^3 + 16h^2 + 6h + 1.$$

This fact have been established by a different way of reasoning in [7]. The equality $W_{\rm avr} = W_{\rm s}$ shows that the Wiener index of any self-linked fibonacene coincides with the average value of the index among all fibonacenes with h rings, i. e. every self-linked fibonacene is an "average" graph of $\mathcal{F}_h$ with respect to the Wiener index.

Corollary 7. *Let $\mathcal{G}_1, \mathcal{G}_2$ be two complete sets of fibonacenes with h rings. Then $W(\mathcal{G}_1)/W(\mathcal{G}_2) = |\,\mathcal{G}_1|/|\,\mathcal{G}_2|$. In particular, $W(\mathcal{G}_1) = W(\mathcal{G}_2)$ if and only if $|\,\mathcal{G}_1| = |\,\mathcal{G}_2|$.*

Applying this result to the set of symmetrical fibonacenes $\mathcal{S}_h$ and to the set of self-linked fibonacenes $\mathcal{L}_h$ with odd number of rings, we have $W(\mathcal{S}_h) = 2W(\mathcal{L}_h)$.

7. Degeneracy of the Wiener index

The set of W-values of hexagonal systems has been subject of detailed investigation since a good ability of an invariant to distinguish between non-isomorphic graphs is important for applications. The discriminating ability of the Wiener index for hexagonal systems was studied in [5, 6, 15, 20, 25].

By a *degeneracy class* we will mean a subset of $\mathcal{F}_h$ consisting of all graphs with the same Wiener index. A *trivial* degeneracy class contains the unique graph. The cardinality of the set $\mathcal{F}_h$ grows as 2^h, while the number of values of $Val(\mathcal{F}_h)$ grows only as h^3. Therefore, for each value of $Val(\mathcal{F}_h)$, the average cardinality of the corresponding degeneracy class has exponential growth. It is well-known that $W(G_1) \equiv W(G_2) \pmod 8$ for arbitrary catacondensed hexagonal systems G_1, G_2 with the same number of rings and W-values of graphs of this class are always odd [13]. The following congruences restrict the possible values of the Wiener index for fibonacenes.

Proposition 8. *For any fibonacenes $G_1, G_2 \in \mathcal{F}_h$,*

1) $W(G_1) \equiv W(G_2) \pmod{16}$ for even h,

2) $W(G_1) \equiv W(G_2) \pmod{32}$ for odd h.

If G_1, G_2 are symmetrical fibonacenes with h rings then

3) $W(G_1) \equiv W(G_2) \pmod{64}$ for odd h.

Proof. All relations follow, for example, from formula (1). Since $h = h_1 + h_2$, any product $h_1 h_2$ is always even for odd h. If G is a symmetrical fibonacene, then u is always even and every product $h_1 h_2$ occurs two times in the sum of formula (1). □

The number of possible values of the Wiener index is $(W_{\max} - W_{\min})/16 + 1 = \binom{h-1}{3} + 1$ for even h and $(W_{\max} - W_{\min})/32 + 1 = \frac{1}{2}\binom{h-1}{3} + 1$ for odd h. The sets of non-realizable values, $[W_{\min}, W_{\min}+16, ..., W_{\max}] \setminus Val(\mathcal{F}_h)$ or $[W_{\min}, W_{\min}+32, ..., W_{\max}] \setminus Val(\mathcal{F}_h)$, are non-empty for every $h \geq 6$.

In studying of topological index degeneracy, a typical problem is to find finite or infinite sets of graphs having the same values of an index. For this purpose, suitable transformations of graphs can be applied. We point out on a simple transformation for fibonacenes. First, return to the transformation shown in Fig. 3b. For such graphs, $W(G) \neq W(H)$ if the subgraphs F_1 and F_2 are non-empty. Suppose that all cut-edges of $C(G)$ have sequentially numbering, $m = |C(B)|$. Consider two cut-edges of G in symmetrical positions with respect to the central edge(s).

Proposition 9. *Let $G \in \mathcal{F}_h$ and edges $e_k \in Z(G)$, $e_{m-k+1} \in U(G)$ or $e_k \in U(G)$, $e_{m-k+1} \in Z(G)$ for fixed $k \in \{1, 2, ..., m\}$. Let a fibonacene H be obtained from G such that $e_k \in U(H)$, $e_{m-k+1} \in Z(H)$ or $e_k \in Z(H)$, $e_{m-k+1} \in U(H)$. Then $W(G) = W(H)$.*

Proof. If two cut-edges of $U(G)$ are in symmetrical positions, then these edges make equal contributions to the sum of formula (1). □

Fibonacenes $G_1, G_2 \in \mathcal{F}_h$ are called W_s-*linked* if $W(G_1) = W(G_2) = W_s$ and G_1, G_2 are linked but non-self-linked graphs, i. e. $G \ncong \overline{G}$. The numbers of W_s-linked graphs for small number of hexagonal rings are shown in Table 1.

Proposition 10. *W_s-linked fibonacenes exist for every odd $h \geq 13$.*

Proof. Suppose that $\mathbf{r}$ and $\bar{\mathbf{r}}$ are codes of W_s-linked fibonacenes with $h-4$ rings. Let $\mathbf{r_1} = (01\mathbf{r}01)$, $\mathbf{r_2} = (10\,\bar{\mathbf{r}}10)$. Then $G_1 = G(\mathbf{r_1})$ and $G_2 = G(\mathbf{r_2})$ are linked but non-self-linked graphs. Since $\mathbf{r}$ and $\bar{\mathbf{r}}$ contain the equal numbers of units, $u(G_1) = u(G_2)$. Cut-edges corresponding to two new units in $\mathbf{r_1}$ and $\mathbf{r_2}$ make equal contributions to the sum of formula (1). Denote by $h_1(e)h_2(e)$ the contribution of an edge e in one of the initial graph with $h-4$ rings. Then this edge makes the following contribution to the corresponding graph with h ring: $(h_1(e)+2)(h_2(e)+2) = h_1(e)h_2(e) + 2h + 4$. This implies that $W(G_1) = W(G_2) = W_s$ (see Proposition 3). The suitable initial graphs have been found for $h = 13, 15$ by computing ($\mathbf{r} = (0001101100)$, $W_s = 11571$ and $\mathbf{r} = (001010110100)$, $W_s = 17191$). □

Proposition 11. *W_s-linked fibonacenes don't exist for $h \equiv 0 \pmod 4$.*

Proof. Suppose that $G, G' \in \mathcal{F}_h$ are W_s-linked fibonacenes and $h \equiv 0 \pmod 4$. Using formula (1) for these graphs, we have

$$[\,u(G)-u(G')\,]\,(h-1)=\sum_{e\in U(G)} h_1(e)h_2(e)-\sum_{e\in U(G')} h_1(e)h_2(e).$$

Since h is even and $u(G)+u(G')=h-3$, the left hand side of the above equation is odd. For the linked graphs G and G', the numbering of cut-edges of $U(G)\cup U(G')$ covers all positions 1,2,...,$h-3$. If a cut edge e is in odd position, then $h_1(e)h_2(e)$ is even, otherwise

Table 1. Degeneracy classes of fibonacenes in $\mathcal{F}_h$.

h — the number of rings of fibonacenes;
$Self$ — the number of self-linked fibonacenes;
W_s — the number of W_s-linked fibonacenes;
Max — the maximal cardinality of degeneracy classes;
Ncl — the number of degeneracy classes;
Ntr — the number of non-trivial degeneracy classes;
Noc — the number of non-trivial degeneracy classes with odd cardinality;
Nec — the number of non-trivial degeneracy classes with even cardinality,
$Ntr = Noc + Nec$.

h	$\|\mathcal{F}_h\|$	$Self$	W_s	Max	Ncl	Ntr	Noc	Nec
4	2	0	0	1	2	0	0	0
5	3	1	0	1	3	0	0	0
6	6	0	0	1	6	0	0	0
7	10	2	0	2	9	1	0	1
8	20	0	0	2	18	2	0	2
9	36	4	0	4	21	11	2	9
10	72	0	2	4	47	19	2	17
11	136	8	0	8	49	35	18	17
12	272	0	0	10	102	68	22	46
13	528	16	4	20	91	73	34	39
14	1056	0	4	20	209	165	76	89
15	2080	32	16	48	155	133	66	67
16	4160	0	0	47	350	314	140	174
17	8256	64	54	118	241	221	94	127
18	16512	0	80	125	547	501	214	287
19	32896	128	184	312	359	339	144	195
20	65792	0	0	312	800	758	334	424
21	131328	256	626	882	505	483	208	275
22	262656	0	430	888	1133	1083	500	583
23	524800	512	1928	2440	699	667	308	359
24	1049600	0	0	2670	1542	1472	658	814
25	2098176	1024	6720	7744	923	889	462	427
26	4196352	0	7788	7813	2029	1969	880	1089
27	8390656	2048	23344	25392	1193	1157	568	589
28	16781312	0	0	24781	2614	2554	1224	1330
29	33558528	4096	74682	78778	1519	1487	730	757
30	67117056	0	57586	80778	3297	3229	1538	1691

$h_1(e)h_2(e)$ is odd. Because of $h \equiv 0 \pmod 4$, the number of even positions is even ($h-3$ is odd). Therefore, the right hand side of the equation is always even. The obtained contradiction implies inequalities $W(G) \neq W(G') \neq W_s$. □

This result demonstrates that there are no fibonacenes of $\mathcal{F}_h$ having Wiener index W_s when $h \equiv 0 \pmod 4$.

The existence of W_s-linked fibonacenes with even number of rings $h \equiv 2 \pmod 4$ is supported by computing (see Table 1) and it is a conjecture for large numbers of rings.

In practice, it is quite difficult to get information about degeneracy classes for graphs with arbitrary number of vertices or rings. Computer calculations are the main tool of investigations of this kind. Some general properties of the degeneracy classes of fibonacenes are collected in the following proposition.

Proposition 12. *For degeneracy classes of fibonacenes $\mathcal{F}_h$,*

(1). *If $h \geq 7$ is odd, then self-linked and W_s-linked fibonacenes form one degeneracy class. Its cardinality equals or more than $2^{(h-5)/2}$ (equality for $h \leq 11$).*

(2). *If $h \geq 10$ is even, then W_s-linked fibonacenes form one degeneracy class when $h \equiv 2 \pmod 4$. The cardinality of this class is even. If $h \equiv 0 \pmod 4$ then W_s is a non-realizable value of the Wiener index (conjecture for large h).*

(3). *If fibonacenes (except of graphs of points (1) and (2)) form a degeneracy class, then their linked graphs also form a degeneracy class with the same cardinality. The numbers of non-trivial degeneracy classes with odd or even cardinality are always even.*

(4). *There are trivial degeneracy classes (helicene, zig-zag fibonacene and others).*

A graphical illustration of this proposition is presented in Fig. 5. Table 1 shows some data of degeneracy classes for fibonacenes with up to 30 rings.

8. Expanding of the Wiener index

Let $\mathbf{Z}_2 = \{0, 1\}$. For binary vectors $\mathbf{x} = (x_1, x_1, ..., x_n)$ and $\mathbf{y} = (y_1, y_1, ..., y_n)$, define two operations: $\mathbf{x}+\mathbf{y} = (x_1+y_1, x_2+y_2, ..., x_n+y_n)$, where $0+0 = 0$ and $0+1 = 1+0 = 1+1 = 1$, and $\lambda \cdot \mathbf{x} = (\lambda \cdot x_1, \lambda \cdot x_2, ..., \lambda \cdot x_n)$ for $\lambda \in \mathbf{Z}_2$, where $0 \cdot 0 = 0 \cdot 1 = 1 \cdot 0 = 0$ and $1 \cdot 1 = 1$. Denote by $\mathbf{e}_i$ the binary vector $\mathbf{e}_i = (0, 0, ..., 0, \overset{i}{1}, 00..., 0)$ of length $h-3$ for positive integer $h \geq 4$. These vectors form the standard basis for the vector space $\mathbf{B}$ of dimension $h-3$ over $\mathbf{Z}_2$.

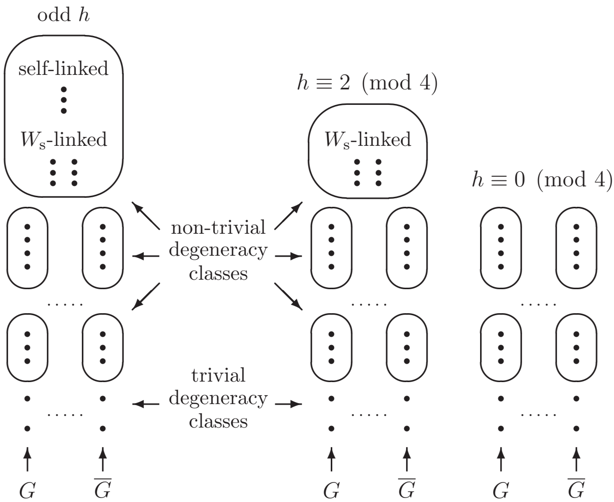

Figure 5. Degeneracy classes of fibonacenes $\mathcal{F}_h$.

In this section, we will consider fibonacenes' codes as vectors. Then a code $\mathbf{r}(G)$ of fibonacene $G \in \mathcal{F}_h$, $h \geq 4$, can be expressed as a linear combination of the basis vectors $\mathbf{e}_i$, $i = 1, 2, ..., h-3$:

$$\mathbf{r}(G) = \lambda_1 \, \mathbf{e}_1 + \lambda_2 \, \mathbf{e}_2 + ... + \lambda_{h-3} \, \mathbf{e}_{h-3},$$

where $\lambda_1, \lambda_2, ..., \lambda_{h-3} \in \mathbf{Z}_2$. For example, fibonacene's code $\mathbf{r}(G) = (00101)$ has the following expanding:

$$\mathbf{r}(G) = (00101) = 0 \cdot \mathbf{e}_1 + 0 \cdot \mathbf{e}_2 + 1 \cdot \mathbf{e}_3 + 0 \cdot \mathbf{e}_4 + 1 \cdot \mathbf{e}_5.$$

In order to get expanding for codes of the helicene H_h or for the zig-zag fibonacene Z_h, one can assume $\lambda_i = 1$ or $\lambda_i = 0$ for all $i = 1, 2, ..., h-3$, respectively.

Denote by F_i the *basis fibonacene* of $\mathcal{F}_h$ corresponding to the basis vector $\mathbf{e}_i$. Since positions of non-zero elements of vectors $\mathbf{e}_i$ and $\mathbf{e}_{h-2-i}$ are symmetrical, $F_i \cong F_{h-2-i}$ for every $i = 1, 2, ..., h-3$. Let $W_i = W(F_i)$.

Proposition 13. *If* $G \in \mathcal{F}_h$ *and* $\mathbf{r}(G) = \lambda_1 \, \mathbf{e}_1 + \lambda_2 \, \mathbf{e}_2 + ... + \lambda_{h-3} \, \mathbf{e}_{h-3}$*, then*

$$W(G) = \lambda_1 W_1 + \lambda_2 W_2 + ... + \lambda_{h-3} W_{h-3} - (u-1) W_{\max},$$

where $u = \lambda_1 + \lambda_2 + ... + \lambda_{h-3} = |U(G)|$.

Proof. Applying formula (1) to every fibonacene F_i, we have

$$W(F_1) = W_{\max} + 16(h-1) - 16\,h_{11}\,h_{12}$$
$$W(F_2) = W_{\max} + 16(h-1) - 16\,h_{21}\,h_{22}$$
$$\vdots$$
$$W(F_{h-3}) = W_{\max} + 16(h-1) - 16\,h_{h-3,1}\,h_{h-3,2}.$$

Multiplying the i-th equation by λ_i for every $i = 1, 2, ..., h-3$ and then summing the obtained equations, we get

$$\sum_{i=1}^{h-3} \lambda_i W_i = (u-1)W_{\max} + W_{\max} + 16u(h-1) - 16 \sum_{e_i \in U(G)} h_{i1}\,h_{i2}.$$

By formula (1), the last three terms in the right hand part of the above equation give the Wiener index of G. □

Assuming $\lambda_i = 1$ for all $i = 1, 2, ..., h-3$, one can calculate the sum of the Wiener indices for all basis graphs F_i.

Corollary 14. *For basis fibonacenes* $F_1, F_2, ..., F_{h-3} \in \mathcal{F}_h$, $h \geq 4$,

$$W_1 + W_2 + ... + W_{h-3} = W_{\min} + (h-4)W_{\max} = \frac{1}{3}(h-3)(16h^3 + 16h^2 + 86h - 37).$$

Proof. Since equalities $\lambda_1 = \lambda_2 = ... = \lambda_{h-3} = 1$ are possible for the helicene only, one can use formula (1) for H_h with $u(H_h) = h-3$. □

Proposition 13 can be applied for the calculating the Wiener indices for subsets of fibonacenes. Let $\mathcal{S}_{h,2k}$ be the set of all symmetrical fibonacenes G with the odd number of rings h and with the numbers of cut-edges $u(G) = 2k$, where $1 \leq k \leq (h-3)/2$. Since the first half of fibonacene's code completely defines the second part, $n = |\mathcal{S}_{h,2k}| = \binom{(h-3)/2}{k}$.

Proposition 15. *For symmetrical fibonacenes of* $\mathcal{S}_{h,2k}$ *with odd* h *and* $u = 2k$,

$$W(\mathcal{S}_{h,2k}) = \binom{(h-5)/2}{k-1}(W_1 + W_2 + ... + W_{h-3}) - \binom{(h-3)/2}{k}(2k-1)W_{\max}.$$

Proof. Applying Proposition 13 to every graph $G_1, G_2, ..., G_n \in \mathcal{S}_{h,2k}$, we have

$$W(G_1) = \lambda_1 W_1 + \lambda_2 W_2 + ... + \lambda_{h-3} W_{h-3} - (2k-1)W_{\max}$$
$$W(G_2) = \lambda_1 W_1 + \lambda_2 W_2 + ... + \lambda_{h-3} W_{h-3} - (2k-1)W_{\max}$$
$$\vdots$$
$$W(G_n) = \lambda_1 W_1 + \lambda_2 W_2 + ... + \lambda_{h-3} W_{h-3} - (2k-1)W_{\max}.$$

It is easy to see that the value $\lambda_i = 1$ occurs $\binom{(h-3)/2-1}{k-1}$ times in the above equalities for every $i = 1, 2, ..., h-3$. The proof is completed by summing these equalities. □

The expression of Proposition 15 can be rewritten in the form

$$W(\mathcal{S}_{h,2k}) = \frac{1}{3k!2^k}(h-3)(h-5)(h-7)(h-9)\cdot ... \cdot(h-2k-1)\phi(h,k),$$

where $\phi(h,k) = 3W_{\max} - 16k(h-1)(h-2)$. For small k, we have the following equalities:

$$W(\mathcal{S}_{h,2}) = (h-3)(16h^3 + 8h^2 + 110h - 53)/6,$$
$$W(\mathcal{S}_{h,4}) = (h-3)(h-5)(16h^3 - 8h^2 + 158h - 85)/24,$$
$$W(\mathcal{S}_{h,6}) = (h-3)(h-5)(h-7)(16h^3 - 24h^2 + 206h - 117)/144.$$

As an illustration, consider symmetrical fibonacenes of $\mathcal{S}_{11,4}$. This set contains 6 graphs with codes (11000011), (10100101), (10011001), (01100110), (01011010), (00111100) and $W(\mathcal{S}_{11,4}) = 7583 + 7455 + 7391 + 7263 + 7199 + 7071 = 43962$. Using Proposition 15, we get $W(\mathcal{S}_{11,4}) = 3 \cdot 64376 - 6 \cdot 3 \cdot 8287 = 43962$.

9. Wiener index for induced fibonacenes

In this section, we consider fibonacenes induced by subsets of arbitrary vectors from the space $\mathbf{B}$ (vectors may induce isomorphic graphs). Vectors $\mathbf{x}$ and $\mathbf{y}$ are called *orthogonal*, $\mathbf{x}\perp\mathbf{y}$, if $\mathbf{x}\cdot\mathbf{y} = \sum_{i=1}^{n} x_i \cdot y_i = 0$. Two vector sets $\mathbf{X}, \mathbf{Y} \subset \mathbf{B}$ are called orthogonal if each vector in $\mathbf{X}$ is orthogonal to each vector in $\mathbf{Y}$. For vectors $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_r\}$, the set of all linear combinations $\{\lambda_1\mathbf{x}_1 + \lambda_2\mathbf{x}_2 + ... + \lambda_r\mathbf{x}_r \mid \lambda_1, \lambda_2, ..., \lambda_r \in \mathbf{Z}_2\}$ is called the *linear hull* of $\mathbf{X}$ and denoted by $\mathcal{H}(\mathbf{X})$. The linear hull is always a vector subspace.

Since binary vectors $\mathbf{r}$ and $\bar{\mathbf{r}}$ induce a fibonacene and its linked graph, $\mathbf{r}\perp\bar{\mathbf{r}}$. Using vectors $\mathbf{r}$ and $\bar{\mathbf{r}}$, one can construct two orthogonal sets of fibonacenes. Namely, if $\mathbf{r} = \mathbf{e}_{i_1} + \mathbf{e}_{i_2} + ... + \mathbf{e}_{i_k}$ and $\bar{\mathbf{r}} = \mathbf{e}_{i_{k+1}} + \mathbf{e}_{i_{k+2}} + ... + \mathbf{e}_{i_{h-3}}$, then the linear hulls $\mathcal{H}(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, ..., \mathbf{e}_{i_k})$ and $\mathcal{H}(\mathbf{e}_{i_{k+1}}, \mathbf{e}_{i_{k+2}}, ..., \mathbf{e}_{i_{h-3}})$ are orthogonal. Consider a set of basis vectors $\mathbf{E} = \{\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, ..., \mathbf{e}_{i_k}\}$ and the corresponding subspace $\mathcal{H}(\mathbf{E})$ with cardinality $n = |\mathcal{H}(\mathbf{E})| = 2^k$, $1 \le k \le h-3$. Let $W(\mathbf{X}) = \sum_{\mathbf{r}\in\mathbf{X}} W(G(\mathbf{r}))$ for a set of vectors $\mathbf{X}$.

Proposition 16. *For the sum of Wiener indices of fibonacenes induced by* $\mathcal{H}(\mathbf{E})$,

$$W(\mathcal{H}(\mathbf{E})) = 2^{k-1}(W_{i_1} + W_{i_2} + ... + W_{i_k}) - 2^{k-1}(k-2)W_{\max}.$$

Proof. Applying Proposition 13 to graphs induced by all vectors $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_n \in \mathcal{H}(\mathbf{E})$, we can write equations for their Wiener indices:

$$\begin{aligned}W(G(\mathbf{r}_1)) &= \lambda_{i_1}W_{i_1} + \lambda_{i_2}W_{i_2} + ... + \lambda_{i_k}W_{i_k} - (u_1-1)W_{\max}\\ W(G(\mathbf{r}_2)) &= \lambda_{i_1}W_{i_1} + \lambda_{i_2}W_{i_2} + ... + \lambda_{i_k}W_{i_k} - (u_2-1)W_{\max}\\ &\vdots\\ W(G(\mathbf{r}_n)) &= \lambda_{i_1}W_{i_1} + \lambda_{i_2}W_{i_2} + ... + \lambda_{i_k}W_{i_k} - (u_n-1)W_{\max}.\end{aligned}$$

The value $\lambda_{i_m} = 1$ occurs 2^{k-1} times in the above equations for every $m = 1, 2, ..., k$. Next, $u_1 + u_2 + ... + u_n = 1\binom{k}{1} + 2\binom{k}{2} + ... + k\binom{k}{k} = k2^{k-1}$. To complete the proof, it is sufficient to sum all equations. □

Let $\mathbf{E}_1 = \{\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, ..., \mathbf{e}_{i_k}\}$, $\mathbf{E}_2 = \{\mathbf{e}_{i_{k+1}}, \mathbf{e}_{i_{k+2}}, ..., \mathbf{e}_{i_{h-3}}\}$ and $\mathbf{E}_1 \cap \mathbf{E}_2 = \emptyset$, $k = (h-3)/2$. Then $\mathcal{H}_1 = \mathcal{H}(\mathbf{E}_1)$ and $\mathcal{H}_2 = \mathcal{H}(\mathbf{E}_2)$ are orthogonal sets with equal cardinalities.

Corollary 17. *For fibonacenes with h rings induced by vectors of $\mathcal{H}_1$ and $\mathcal{H}_2$, $h \geq 5$,*

$$W(\mathcal{H}_1) + W(\mathcal{H}_2) = 2^{(h-5)/2}\left(W_1 + W_2 + ... + W_{h-3} - (h-7)W_{\max}\right).$$

Consider vector sets $\mathbf{E}_1 = \{(1000), (0001)\}$ and $\mathbf{E}_2 = \{(0100), (0010)\}$, $h = 7$. Then $\mathcal{H}_1 = \{(0000), (1000), (0001), (1001)\}$ and $\mathcal{H}_2 = \{(0000), (0100), (0010), (0110)\}$. By computer calculations, $W(\mathcal{H}_1) = 2359 + 2295 + 2295 + 2231 = 9180$ and $W(\mathcal{H}_2) = 2359 + 2263 + 2263 + 2167 = 9052$. From Corollary 17, we have $W(\mathcal{H}_1) + W(\mathcal{H}_2) = 2(W_1 + W_2 + W_3 + W_4) = 2(2295 + 2263 + 2263 + 2295) = 18232$.

If a set $\mathbf{E}$ contains all basis vectors, $\mathcal{H}(\mathbf{E}) = \mathbf{B}$.

Corollary 18. *For fibonacenes with h rings induced by all vectors of* $\mathbf{B}$,

$$W(\mathbf{B}) = 2^{h-3}\left(4h^3 + 16h^2 + 6h + 1\right) = |\mathbf{B}|\, W_{\mathrm{s}}.$$

Proof. By Propositions 16 and Corollary 14, we have

$$\begin{aligned}W(\mathbf{B}) &= 2^{h-4}(h-3)(16h^3 + 16h^2 + 86h - 37)/3\\ &\quad - 2^{k-4}(k-5)(16h^3 + 24h^2 + 62h - 21)/3\\ &= 2^{h-4}(8h^3 + 32h^2 + 12h + 2) = 2^{h-3}(4h^3 + 16h^2 + 6h + 1). \quad \square\end{aligned}$$

Corollary 18 follows also from a fact that the set of fibonacenes induced by all vectors of $\mathbf{B}$ is complete.

Let $\mathbf{X}_{h,k}$ be the set of vectors of length $h-3$ with k units, $|\mathbf{X}_{h,k}| = \binom{h-3}{k}$. For example, $\mathbf{X}_{h,1}$ induces all basis fibonacenes and the helicene is induced by $\mathbf{X}_{h,h-3}$.

Proposition 19. *For the Wiener index of fibonacenes induced by $\mathbf{X}_{h,k}$,*

$$W(\mathbf{X}_{h,k}) = \binom{h-4}{k-1}(W_1 + W_2 + ... + W_{h-3}) - \binom{h-3}{k}(k-1)W_{\max}.$$

Proof. Applying Proposition 13 to graphs $\mathbf{r}(G_1), \mathbf{r}(G_2), ..., \mathbf{r}(G_n)$, we get

$$\begin{aligned} W(\mathbf{r}(G_1)) &= \lambda_1 W_1 + \lambda_2 W_2 + ... + \lambda_{h-3} W_{h-3} - (k-1) W_{\max} \\ W(\mathbf{r}(G_2)) &= \lambda_1 W_1 + \lambda_2 W_2 + ... + \lambda_{h-3} W_{h-3} - (k-1) W_{\max} \\ &\vdots \\ W(\mathbf{r}(G_n)) &= \lambda_1 W_1 + \lambda_2 W_2 + ... + \lambda_{h-3} W_{h-3} - (k-1) W_{\max}. \end{aligned}$$

The value $\lambda_i = 1$ occurs $\binom{h-4}{k-1}$ times in the above equations for every $i = 1, 2, ..., h-3$. □

The equality of the above proposition can be written in the form

$$W(\mathbf{X}_{h,k}) = \frac{1}{3k!}(h-3)(h-4)(h-5)(h-6) \cdot ... \cdot (h-k-2)\phi(h,k),$$

where $\phi(h,k) = 3W_{\max} - 8k(h-1)(h-2)$. For small k, we have the following equalities:

$$\begin{aligned} W(\mathbf{X}_{h,2}) &= (h-3)(h-4)(16h^3 + 8h^2 + 110h - 53)/6, \\ W(\mathbf{X}_{h,3}) &= (h-3)(h-4)(h-5)(16h^3 + 134h - 69)/18, \\ W(\mathbf{X}_{h,4}) &= (h-3)(h-4)(h-5)(h-6)(16h^3 - 8h^2 + 158h - 85)/72. \end{aligned}$$

Consider set $\mathbf{X}_{7,2} = \{(1100), (1010), (1001), (0110), (0101), (0011)\}$. Then $W(\mathbf{X}_{7,2}) = 2199 + 2199 + 2231 + 2167 + 2199 + 2199 = 13194$. By the above formula for $k = 2$, we have $W(\mathbf{X}_{7,2}) = (4 \cdot 3 \cdot 6597)/6 = 13194$.

From Proposition 15 and 19, we can obtain a relation between the Wiener indices of symmetrical fibonacenes $\mathcal{S}_{h,2k} \subseteq \mathcal{F}_h$ and fibonacenes induced by the vector set $\mathbf{X}_{h,2k}$: $3W(\mathbf{X}_{h,2k}) = (h-4)(h-6) \cdot ... \cdot (h-2k-2)W(\mathcal{S}_{h,2k})$.

Let $\mathbf{X} = \{\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{h-3}\} \subseteq \mathbf{B}$ and $\mathbf{r}_2, \mathbf{r}_3, ..., \mathbf{r}_{h-3}$ be obtained from the vector $\mathbf{r}_1$ of length $h-3$ by cyclic shifts of its units. These vectors induce $h-3$ fibonacenes with the same numbers of cut-edges $u = u(G(\mathbf{r}_1)) = ... = u(G(\mathbf{r}_{h-3}))$. Suppose that the value of $W(\mathbf{X})$ is known and we are interesting in the following question: how to find the number of cut-edges u in the induced graphs?

Proposition 20. *For the number of cut-edges of fibonacenes $G(\mathbf{r}_1), G(\mathbf{r}_2), ..., G(\mathbf{r}_{h-3})$,*

$$u = \frac{1}{16}\binom{h-1}{3}^{-1}\Big((h-3)W_{\max} - W(\mathbf{X})\Big).$$

Proof. Applying Proposition 13 to graph $G(\mathbf{r}_i)$ for every $i = 1, 2, ..., h-3$ and then summing all equalities, we have

$$W(\mathbf{X}) = u(W_1 + W_2 + ... + W_{h-3}) - (h-3)(u-1)W_{\max}.$$

After simplification, we obtain the number of cut-edges in the induced graphs. □

As an illustration, consider vector $\mathbf{r}_1 = (001011)$. Then $\mathbf{r}_2 = (100101)$, $\mathbf{r}_3 = (110010)$, $\mathbf{r}_4 = (011001)$, $\mathbf{r}_5 = (101100)$, and $\mathbf{r}_6 = (010110)$. Computer calculating of the Wiener indices gives $W(\mathbf{X}) = 25602$. By Proposition 20, we can write

$$u = \frac{1}{16} \cdot \frac{1}{56} \left(6 \cdot 4715 - 25602\right) = \frac{1}{896} \left(28290 - 25602\right) = 3.$$

Remark 1. It is well known that the Wiener index of a tree T with n vertices can be calculated through eigenvalues $\lambda_1 \geq ... \geq \lambda_{n-1}$ of Laplacian matrix of T [21]:

$$W(T) = \frac{1}{n} \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \cdots + \frac{1}{\lambda_{n-1}} \right).$$

This implies that Laplacian eigenvalues of a branching tree define the Wiener index of the corresponding fibonacene G with h rings, $W(G) = f(h, \lambda_1, \ldots, \lambda_{n-1})$.

Remark 2. There are explicit relations between the Wiener index and some topological indices of fibonacenes $G \in \mathcal{F}_h$. For the Schultz molecular topological index [7], $MTI(G) = 5W(G) - (12h^2 - 14h + 5)$. It is easy to verify that for the Szeged index [18], $Sz(G) = 3W(G) - (16h^3 + 24h^2 + 158h - 36)/6$. This implies that the Wiener index and these indices have the similar collective properties.

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