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On the Wiener Index of Certain Families 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 form a class of unbranched catacondensed benzenoid hydrocarbons having zig-zag structure. Collective properties of the Wiener index for some classes of fibonacenes have been studied in [4]. We present new families of fibonacenes for which the sum of their Wiener indices can be easily calculated.

1. Introduction

In this paper we are concerned with finite undirected connected graphs. The vertex set of G is denoted by $V(G)$. 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 [19]. It is defined as the sum of distances between all unordered pairs of vertices of a graph G:

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

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

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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 [3, 8, 11, 12, 17, 18] and reviews [5, 6, 13, 14, 15, 16].

In this paper we study the Wiener index for hexagonal chains 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 graph, but a collective property of sets of such graphs. This approach may be useful in studying of topological indices of molecular graphs or in characterizing sets of graphs obtained after destruction of hexagonal networks. Some results in this direction have been reported in [4].

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, 4, 9, 10].

Denote by $\mathcal{F}_h$ the set of all fibonacenes with h rings. Throughout this article h always denotes the number of hexagonal rings in a graph.

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.

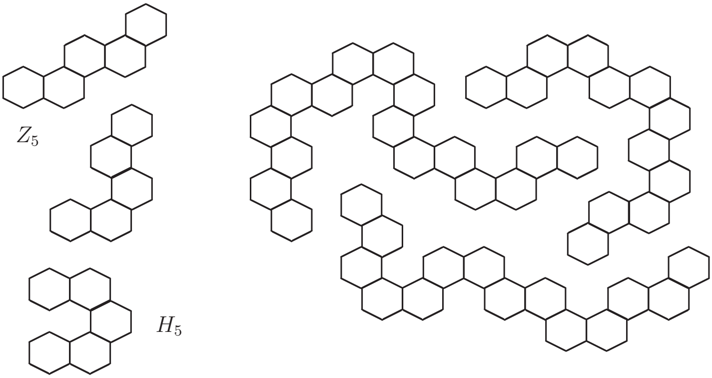


Figure 1: Three small and three large fibonacenes.

3. Representation of fibonacenes

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). 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, $|C(G)| = h - 3$. This set can be decomposed into two disjoint subsets: $C(G) = U(G) \cup Z(G)$. Namely, suppose that all cut-edges of G are sequentially numbered by 0, 1, 2,...,$h-2$. For a cut-edge $e_i \in C(G)$, consider a subgraph P_i with four hexagons containing cut-edges $\{e_{i-1}, e_i, e_{i+1}\}$, $1 \leq i \leq h-3$. Subgraph P_i is isomorphic to helicene H_4 or to zig-zag fibonacene Z_4 for every $i = 1, 2, ..., h-3$ (see Fig. 2). We assume that $e_i \in U(G)$ if $P_i \cong H_4$ and $e_i \in Z(G)$ if $P_i \cong Z_4$. Denote by $u(G)$ the cardinality of $U(G)$.

The structure of an arbitrary fibonacene $G \in \mathcal{F}_h$ can be represented as a binary code $\mathbf{r}(G) = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{h-3})$. If a cut-edge e_i belongs to $U(G)$ then $\mathbf{r}_i = 1$, otherwise $\mathbf{r}_i = 0$, $i = 1, 2, ..., h-3$ (see Fig. 2). A fibonacene with non-trivial symmetry has a symmetrical code. For instance, the most right large fibonacene in Fig. 1 has the following code: (010010010). Denote by $\mathcal{S}_h$ the set of all symmetrical fibonacenes with h rings.

A fibonacene induced by a binary vector $\mathbf{r}$ will be denoted by $G(\mathbf{r})$. Components of a *reverse code* $\mathbf{r}^*$ of a code $\mathbf{r}$ are defined as ${\mathbf{r}^*}_i = \mathbf{r}_{h-2-i}$, $1 \leq i \leq h-3$. It is clear that fibonacenes $G(\mathbf{r})$ and $G(\mathbf{r}^*)$ are always isomorphic. We will assume that $\mathbf{r}(G)$ corresponds to one of two possible codes of G (it is not important how to choose $\mathbf{r}(G)$).

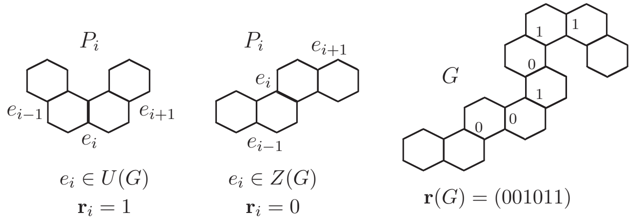


Figure 2: Binary representation of fibonacenes.

All codes of a family of graphs $\mathcal{G}_h = \{G(\mathbf{r}_1), G(\mathbf{r}_2), ..., G(\mathbf{r}_k)\}$ with h rings form the binary $k \times (h-3)$ matrix $\mathbf{M}(\mathcal{G}_h)$ with rows $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_k$. The complement of a family $\mathcal{G}_h$ is defined as $\overline{\mathcal{G}}_h = \{G(\overline{\mathbf{r}}_1), G(\overline{\mathbf{r}}_2), ..., G(\overline{\mathbf{r}}_k)\}$, where $\overline{\mathbf{r}}$ denotes the bitwise negation of $\mathbf{r}$.

4. Linked fibonacenes

By family of fibonacenes we mean a multiset, *i.e.* a family may contain isomorphic graphs. A family or set of fibonacenes $\mathcal{G}_h = \{G_1, G_2, ..., G_k\}$ is called *m-linked* if every column of the matrix $\mathbf{M}(\mathcal{G}_h)$ contains exactly m units, *i.e.* $\mathbf{r}_i(G_1)+\mathbf{r}_i(G_2)+...\mathbf{r}_i(G_k) = m$ for every $i = 1, 2, ..., h-3$. An example of such a family is shown in Fig. 3.

Let $\mathcal{G}_h$ be a m-linked family of fibonacenes and $|\mathcal{G}_h| = k$. If $m = 0$ and $k \geq 1$ then $\mathcal{G}_h$ contains k zig-zag fibonacenes Z_h. If $m = k$ then $\mathcal{G}_h$ contains k helicenes H_h. If $Z_h \notin \mathcal{G}_h$ then $m \leq |\mathcal{G}_h| \leq m(h-3)$.

Let $\mathcal{G}$, $\mathcal{G}'$ be arbitrary m-linked and m'-linked families of fibonacenes, respectively. It is clear that $\mathcal{G} \cup \mathcal{G}'$ is always $(m+m')$-linked family. If $\mathcal{G} \cap \mathcal{G}'$ is a m''-linked family then $\mathcal{G} \setminus \mathcal{G}'$ is $(m-m'')$-linked family. The complement $\overline{\mathcal{G}}$ is a $(k-m)$-linked family if $|\mathcal{G}| = k$.

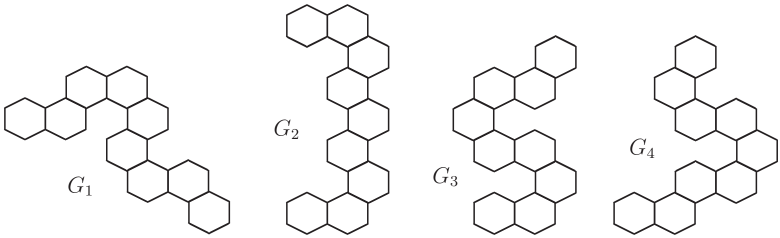
The notion of linked fibonacenes has been introduced in [4]: two graphs $G(\mathbf{r})$ and $G'(\mathbf{r}')$ are linked if $\mathbf{r}' = \overline{\mathbf{r}}$ and a fibonacene G is *self-linked* if $G(\mathbf{r}) \cong G(\overline{\mathbf{r}})$. Self-linked fibonacenes exist if their number of rings h is odd. A set of fibonacenes $\mathcal{G}$ is called *complete* if for every fibonacene $G \in \mathcal{G}$ the set always contains its linked graph $\overline{G}$ [4].

Examples.

1. A fibonacene G and its linked graph $\overline{G}$ always form a 1-linked set.

2. Any complete set of fibonacenes $\mathcal{G}_h$ is $|\mathcal{G}_h|/2-$linked, $\mathcal{G}_h = \cup\{G, \overline{G}\}$.

3. The set of all symmetrical fibonacenes $\mathcal{S}_h$ is $|\mathcal{S}_h|/2-$linked. Indeed, this set can be also represented as union of disjoint 1-linked sets $\{G, \overline{G}\}$, *i.e.* $\mathcal{S}_h$ is a complete set.



$\mathbf{r}(G_1) = (011010)$ $\mathbf{r}(G_2) = (100001)$ $\mathbf{r}(G_3) = (110110)$ $\mathbf{r}(G_4) = (001101)$

$$\mathcal{G}_9 = \{G_1, G_2, G_3, G_4\}, \ \ M(\mathcal{G}_9) = \begin{bmatrix} \mathbf{r}(G_1) \\ \mathbf{r}(G_2) \\ \mathbf{r}(G_3) \\ \mathbf{r}(G_4) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \end{bmatrix}.$$

Figure 3: 2-linked family of fibonacenes $\mathcal{G}_9$.

4. The set of all fibonacenes is $|\mathcal{F}_h|/2$– linked for even h, $\mathcal{F}_h = \cup\{G, \overline{G}\}$. Let $\mathcal{L}_h \subset \mathcal{F}_h$ be the set of all self-linked fibonacenes for odd h. Then $\mathcal{F'}_h = \mathcal{F}_h \setminus \mathcal{L}_h = \cup\{G, \overline{G}\}$ is a $|\mathcal{F'}_h|/2$– linked set.

5. Let $\mathcal{B}_h$ be a family of fibonacenes induced by all binary vectors of length $h-3$. Since $\mathcal{B}_h = \cup\{G, \overline{G}\}$, $\mathcal{B}_h$ is a $|\mathcal{B}_h|/2$– linked family.

6. Let $G \in \mathcal{F}_h$ be an arbitrary fibonacene and $\mathbf{r}(G)$ has m units. Then the family generated by all cyclic shifts of bits in $\mathbf{r}(G)$ is m-linked.

5. Wiener index of linked fibonacenes

It is known that Wiener indices of helicene H_h and zig-zag fibonacene Z_h are the minimal and the maximal W-values among all fibonacenes [2, 7]:

$$W_{\min} = W(H_h) = \frac{1}{3}\left(8h^3 + 72h^2 - 26h + 27\right),$$
$$W_{\max} = W(Z_h) = \frac{1}{3}\left(16h^3 + 24h^2 + 62h - 21\right),$$
$$W_{\max} - W_{\min} = 16\binom{h-1}{3}.$$

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

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

Further, these W-values will be considered only for graphs with h rings. The sum of the Wiener indices for all fibonacenes $G \in \mathcal{G}$ will be denoted by $W(\mathcal{G}) = \sum_{G\in\mathcal{G}} W(G)$.

Let $e \in U(G)$ be a cut-edge of $G \in \mathcal{G}_h$ and $u = |U(G)|$. Denote by $l(e)$ and $r(e)$ the numbers of rings of two fibonacenes obtained by cutting G along the edge e, $l(e)+r(e) = h$. To calculate the Wiener index of an arbitrary fibonacene G, it is sufficient to examine its cut-edges from $U(G)$ [4]:

$$W(G) = W_{\max} + 16\,u(h-1) - 16 \sum_{e\in U(G)} l(e)r(e). \tag{1}$$

The following result shows how to calculate the Wiener index for a m-linked family of fibonacenes.

Proposition 1. *For an arbitrary m-linked family of fibonacenes $\mathcal{G}_h = \{G_1, G_2, ..., G_k\}$,*

$$\begin{aligned} W(\mathcal{G}_h) &= |\,\mathcal{G}_h|\,W_{\max} - m(W_{\max} - W_{\min}) \\ &= |\,\mathcal{G}_h|\,W_{\max} - 16m\binom{h-1}{3} \\ &= \tfrac{1}{3}\left(8h^3(2k-m) + 24h^2(k+2m) + 2h(31k-44m) - 3(7k-16m)\right). \end{aligned}$$

Proof. Let $u_i = |\,U(G_i)|$, $i = 1, 2, ..., k$. Applying formula (1) to every fibonacene of $\mathcal{G}_h$, we have

$$W(\mathcal{G}_h) = kW_{\max} + 16(u_1 + u_2 + ... + u_k)(h-1) - 16 \sum_{e\in U_1\cup...\cup U_k} l(e)r(e).$$

Since $\mathcal{G}_h$ is a m-linked family, $u_1 + u_2 + ... + u_k = m(h-3) = m\,u(H_h)$ and

$$\sum_{e\in U_1\cup...\cup U_k} l(e)r(e) = m \sum_{e\in U(H_h)} l(e)r(e).$$

Then $W(\mathcal{G}_h) = (k-m)W_{\max} + mW(H_h)$ and Proposition 1 follows. $\square$

For graphs in Fig. 3, $W(\mathcal{G}_9) = 4203+4523+4107+4235 = 17068 = 4\cdot 4715-16\cdot 2\binom{9-1}{3}$.

Corollary 2. [4] *For an arbitrary fibonacene $G \in \mathcal{G}_h$,*

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

Corollary 3. *Let $\mathcal{G}_h$ and $\mathcal{G}'_h$ be m-linked families of fibonacenes with h rings. Then $W(\mathcal{G}_h) = W(\mathcal{G}'_h)$ if and only if $|\,\mathcal{G}_h| = |\,\mathcal{G}'_h|$.*

Proof. By Proposition 1, we have $W(\mathcal{G}_h) - W(\mathcal{G}'_h) = W_{\max}(|\,\mathcal{G}_h| - |\,\mathcal{G}'_h|)$. $\square$

Corollary 4. *For an arbitrary $|\mathcal{G}_h|/2$–linked family of fibonacenes $\mathcal{G}_h$,*

$$W(\mathcal{G}_h) = |\mathcal{G}_h|\, W_s.$$

Proof. By Proposition 1, we can write $W(\mathcal{G}_h) = |\mathcal{G}_h|\, W_{\max} - \frac{|\mathcal{G}_h|}{2}(W_{\max} - W_{\min}) = |\mathcal{G}_h|\,(W_{\max} + W_{\min})/2 = |\mathcal{G}_h|\, W_s$. □

Since the set of all fibonacenes $\mathcal{F}_h$ with odd h contains the subset $\mathcal{L}_h$ of self-linked graphs, $\mathcal{F}_h$ is not $|\mathcal{F}_h|/2$– linked. However, it is known that for any $G \in \mathcal{L}_h$ the equality $W(G) = W_s$ holds (see Corollary 2). Then $W(\mathcal{F}_h) = |\mathcal{F}_h|\, W_s$ also for odd h.

Examples.

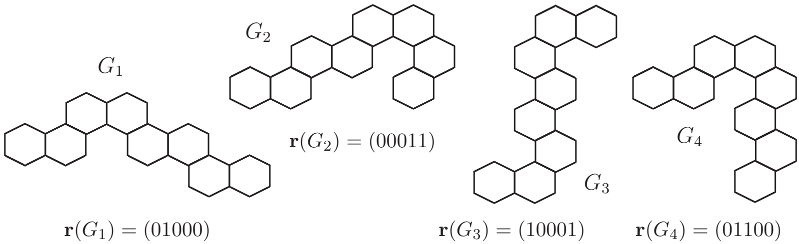
1. Let $\mathcal{G}_h$ be a family of fibonacenes with odd h induced by all binary vectors of length $h-3$ having $\frac{h-3}{2}$ units. The cardinality of this family is equal to $\binom{h-3}{\frac{1}{2}(h-3)}$. The number of graphs $G \in \mathcal{G}_h$ with $\mathbf{r}_i(G) = 1$ for every fixed $i = 1, 2, ..., h-3$ is equal to $\binom{h-4}{\frac{1}{2}(h-5)}$. Therefore, $\mathcal{G}_h$ is a $\binom{h-4}{\frac{1}{2}(h-5)}$–linked family. Since $\binom{h-4}{\frac{1}{2}(h-5)} = \frac{1}{2}\binom{h-3}{\frac{1}{2}(h-3)}$, we can apply Corollary 4. Therefore, $W(\mathcal{G}_h) = |\mathcal{G}_h|\, W_s = \binom{h-3}{\frac{1}{2}(h-3)} W_s$.

2. By distance $d_H(G_1, G_2)$ between fibonacenes G_1 and G_2 we mean Hamming distance $d_H(\mathbf{r}(G_1), \mathbf{r}(G_2))$ between their binary codes $\mathbf{r}(G_1)$ and $\mathbf{r}(G_2)$, *i.e.* $d_H(G_1, G_2)$ is equal to the number of codes' components for which $\mathbf{r}_i(G_1) \neq \mathbf{r}_i(G_2)$, $i = 1, 2, ..., h-3$.

Denote by $S(G_0)$ the sphere of radius 1 with the center in a fibonacene G_0: $S(G_0) = \{G \in \mathcal{F}_h \,|\, d_H(G_0, G) = 1\}$, $|S(G_0)| = h-3$. It is clear that $S(\overline{G}) = \overline{S(G)}$. Therefore, $S(G) \cup S(\overline{G})$ is a complete set of fibonacenes and $W(S(G) \cup S(\overline{G})) = 2(h-3)W_s$.

6. Symmetrically linked fibonacenes

In this section, we define more general families of fibonacenes $\mathcal{G}_h = \{G_1, G_2, ..., G_k\}$ which include linked families. Let $\mathbf{M}(\mathcal{G}_h) = [m_{i,j}]$, $i = 1, 2, ..., k$, $j = 1, 2, ..., h-3$. Columns j_1 and j_2 of $\mathbf{M}(\mathcal{G}_h)$ are called *symmetrical* if $j_2 = h-2-j_1$ for $1 \leq j_1 \leq \lfloor \frac{h-3}{2} \rfloor$. A family of fibonacenes $\mathcal{G}_h$ is called *symmetrically a-linked* if the sum of units in every pairs of symmetrical columns of $\mathbf{M}(\mathcal{G}_h)$ is equal to a (if h is even then the central column does not take into account), *i.e.* $a = \sum_{i=1}^{k} m_{i,j} + \sum_{i=1}^{k} m_{i,h-2-j}$ for every $j = 1, 2, ..., \lfloor \frac{h-3}{2} \rfloor$ and $a \leq 2k$. It is clear that a m-linked family is always symmetrically $2m$-linked. An example of such a family is shown in Fig. 4.



$$\mathcal{G}_8 = \{G_1, G_2, G_3, G_4\}, \quad M(\mathcal{G}_8) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 \end{bmatrix}.$$

Figure 4: Symmetrically 3-linked family of fibonacenes $\mathcal{G}_8$.

Proposition 6. *For an arbitrary symmetrically a-linked family of fibonacenes $\mathcal{G}_h$ (with b units in the central column of $\mathbf{M}(\mathcal{G}_h)$ for even h),*

$$W(\mathcal{G}_h) = |\,\mathcal{G}_h|\, W_{\max} - 8a\binom{h-1}{3} - \phi(a,b),$$

where $\phi(a,b) = 0$ for odd h and $\phi(a,b) = 2(h-2)^2(2b-a)$ for even h.

Proof. To calculate $W(\mathcal{G}_h)$, we apply formula (1). Denote by c_i the sum of units in i-th column of $\mathbf{M}(\mathcal{G}_h)$. For $e_i \in U(G)$, we shall write $l(e_i) = l_i$ and $r(e_i) = r_i$. Let h be even. Then

$$\begin{aligned} \textstyle\sum_{G\in\mathcal{G}_h} u(G) &= c_1 + c_2 + ... + c_{h-3} \\ &= (c_1 + c_{h-3}) + (c_2 + c_{h-4}) + ... + (c_{\frac{h-4}{2}} + c_{\frac{h}{2}}) + c_{\frac{h-2}{2}} \\ &= \tfrac{1}{2}a(h-4) + b = \tfrac{1}{2}u(H_h) - \tfrac{1}{2}a + b. \end{aligned}$$

Since $l_{\frac{h-2}{2}} = r_{\frac{h-2}{2}} = \frac{h}{2}$,

$$\textstyle\sum_{G\in\mathcal{G}_h} \sum_{e\in U(G)} l(e)r(e) = c_1\, l_1\, r_1 + c_2\, l_2\, r_2 + ... + c_{h-3}\, l_{h-3}\, r_{h-3}$$

$$= l_1\, r_1\, [\, c_1 + c_{h-3}\,] + l_2\, r_2\, [\, c_2 + c_{h-4}\,] + ... + l_{\frac{h-4}{2}}\, r_{\frac{h-4}{2}}\, [\, c_{\frac{h-4}{2}} + c_{\frac{h}{2}}\,] + c_{\frac{h-2}{2}}\, l_{\frac{h-2}{2}}\, r_{\frac{h-2}{2}}$$

$$= a[\, l_1\, r_1 + l_2\, r_2 + ... + l_{\frac{h-4}{2}}\, r_{\frac{h-4}{2}}\,] + b\, l_{\frac{h-2}{2}}\, r_{\frac{h-2}{2}}$$

$$= \tfrac{1}{2}a \textstyle\sum_{e\in U(H_h)} l(e)r(e) - \tfrac{1}{2}a\, l_{\frac{h-2}{2}}\, r_{\frac{h-2}{2}} + b\, l_{\frac{h-2}{2}}\, r_{\frac{h-2}{2}}$$

$$= \tfrac{1}{2}a \textstyle\sum_{e\in U(H_h)} l(e)r(e) - \tfrac{1}{8}ah^2 + \tfrac{1}{4}bh^2.$$

Substituting these equalities into formula (1), we get Proposition 6. For odd h, all calculations are almost the same. □

For the family of fibonacenes in Fig. 4, we have $a = 3$, $b = 1$, and $W(\mathcal{G}_8) = 3273 + 3193 + 3241 + 3129 = 12836 = 4 \cdot 3401 - 8 \cdot 3\binom{8-1}{3} - 2(8-2)^2(2-3)$.

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