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TOPOLOGICAL INDICES FOR THE ANTIREGULAR GRAPHS

E. MUNARINI

We determine some classical distance-based and degree-based topological indices of the connected antiregular graphs (maximally irregular graphs). More precisely, we obtain explicitly the k-Wiener index, the hyper-Wiener index, the degree distance, the Gutman index, the first, second and third Zagreb index, the reduced first and second Zagreb index, the forgotten Zagreb index, the hyper-Zagreb index, the refined Zagreb index, the Bell index, the min-deg index, the max-deg index, the symmetric division index, the harmonic index, the inverse sum indeg index, the M-polynomial and the Zagreb polynomial.

1. Introduction

In chemical graph theory, there are several distance-based or degree-based topological indices used to describe the structure of a connected graph $G = (V,E)$. The most common distance-based indices are the *k-Wiener indices*

$$\mathcal{W}_k(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)^k = \frac{1}{2}\sum_{u,v\in V(G)} d(u,v)^k \qquad (k \in \mathbb{Z})$$

where the first sum is over all pairs of distinct vertices of G, while the second sum is over all ordered pairs of vertices of G. For $k = 1$, we have the original

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Wiener index, $\mathcal{W}(G) = \mathcal{W}_1(G)$, introduced by Wiener in 1947 in order to determine the boiling point of paraffins [47, 48]. For $k = -1$, we have the *Harary index* [29, 39, 50, 52], $\mathcal{H}(G) = \mathcal{W}_{-1}(G)$. Another index of this kind is the *hyper-Wiener index* [30, 40], defined by

$$\mathcal{WW}(G) = \frac{1}{2}\big(\mathcal{W}_1(G) + \mathcal{W}_2(G)\big).$$

Two classical generalizations of the Wiener index are the *degree distance* [7, 22], defined by

$$\mathcal{D}(G) = \sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))d(u,v) = \frac{1}{2}\sum_{u,v\in V(G)} (d(u)+d(v))d(u,v),$$

and the *Gutman index* [22], defined by

$$\mathrm{Gut}(G) = \sum_{\{u,v\}\subseteq V(G)} d(u)d(v)d(u,v) = \frac{1}{2}\sum_{u,v\in V(G)} d(u)d(v)d(u,v).$$

Two of the oldest degree-based topological indices are the *first* and *second Zagreb index* [26, 27], defined by

$$\begin{aligned} M_1(G) &= \sum_{\{v,w\}\in E(G)} (d(v)+d(w)) = \sum_{v\in V(G)} d(v)^2 \\ M_2(G) &= \sum_{\{v,w\}\in E(G)} d(v)d(w). \end{aligned}$$

In addition to these classical indices, we have a huge host of other degree-based descriptors [17, 23, 46]. For instance, we have the *third Zagreb index* (or *Albertson index*, or *irregularity*) [2, 11, 12]

$$\begin{aligned} M_3(G) &= \sum_{\{v,w\}\in E(G)} |d(v)-d(w)| \\ &= \sum_{\{v,w\}\in E(G)} (\max(d(v),d(w)) - \min(d(v),d(w))), \end{aligned}$$

the *reduced first Zagreb index* [8]

$$\mathrm{RM}_1(G) = \sum_{v\in V(G)} (d(v)-1)^2 = M_1(G) + |V(G)| - 4|E(G)|,$$

the *reduced second Zagreb index*[1] [16]

$$\mathrm{RM}_2(G) = \sum_{\{u,v\}\in E(G)} (d(u)-1)(d(v)-1)$$

[1] See [18, 52] for some recent results on these indices.

and the *difference of Zagreb indices* $\Delta\mathrm{M}(G) = M_2(G) - M_1(G)$, related by the identity

$$\mathrm{RM}_2(G) = \Delta\mathrm{M}(G) + |E(G)|\,,$$

the *forgotten Zagreb index* (or *F-index*) [15, 17]

$$F(G) = \sum_{\{v,w\}\in E(G)} (d(v)^2 + d(w)^2) = \sum_{v\in V(G)} d(v)^3\,,$$

the *hyper-Zagreb index* [44]

$$HM(G) = \sum_{\{v,w\}\in E(G)} (d(v) + d(w))^2 = F(G) + 2M_2(G)\,,$$

the *refined Zagreb index*

$$r(G) = \sum_{\{v,w\}\in E(G)} d(v)d(w)(d(v) + d(w))\,,$$

the *Bell index* [3, 17]

$$B(G) = \sum_{v\in V(G)} \left(d(v) - 2\frac{|E(G)|}{|V(G)|}\right)^2 = M_1(G) - 4\frac{|E(G)|^2}{|V(G)|}$$

and the associated *variance of the vertex degrees* [3]

$$\mathrm{Var}(G) = \frac{1}{|V(G)|}\sum_{v\in V(G)} d(v)^2 - \frac{1}{|V(G)|^2}\left(\sum_{v\in V(G)} d(v)\right)^2 = \frac{B(G)}{|V(G)|}\,,$$

the *min-deg index* and the *max-deg index*

$$\mathrm{M}_{\min}(G) = \sum_{\{v,w\}\in E(G)} \min(d(v), d(w))$$
$$\mathrm{M}_{\max}(G) = \sum_{\{v,w\}\in E(G)} \max(d(v), d(w))\,,$$

the *symmetric division index* [20, 21]

$$\begin{aligned}\mathrm{SSD}(G) &= \sum_{\{v,w\}\in E(G)} \left(\frac{\min(d(v), d(w))}{\max(d(v), d(w))} + \frac{\max(d(v), d(w))}{\min(d(v), d(w))}\right)\\ &= \sum_{\{v,w\}\in E(G)} \left(\frac{d(v)}{d(w)} + \frac{d(w)}{d(v)}\right) = \sum_{\{v,w\}\in E(G)} \frac{d(v)^2 + d(w)^2}{d(v)d(w)}\,.\end{aligned}$$

Other two similar descriptors are the *harmonic index* [9, 13, 23, 53–55]

$$h(G) = \sum_{\{v,w\} \in E(G)} \frac{2}{d(v)+d(w)}$$

and the *inverse sum index* (or *inverse sum indeg index*) [38, 43, 46]

$$I(G) = \sum_{\{v,w\} \in E(G)} \frac{1}{\frac{1}{d(v)} + \frac{1}{d(w)}} = \sum_{\{v,w\} \in E(G)} \frac{d(v)d(w)}{d(v)+d(w)}\,.$$

A natural generalization of these indices is the *M-polynomial* [6]

$$M(G;x,y) = \sum_{\substack{\{v,w\} \in E(G) \\ d(v) \leq d(w)}} x^{d(v)} y^{d(w)} = \sum_{\{v,w\} \in E(G)} x^{\min(d(v),d(w))} y^{\max(d(v),d(w))} \tag{1}$$

or the *symmetric Zagreb polynomial*

$$Z(G;x,y) = M(G;x,y) + M(G;y,x) = \sum_{\{v,w\} \in E(G)} \left(x^{d(v)} y^{d(w)} + x^{d(w)} y^{d(v)}\right). \tag{2}$$

For $x = y = q$, we have the (*first*) *Zagreb polynomial* [5, 10, 25]

$$Z(G;q) = \frac{1}{2} Z(G;q,q) = \sum_{\{v,w\} \in E(G)} q^{d(v)+d(w)}\,. \tag{3}$$

The previous distance-based descriptors can be retrieved from these polynomials. For instance, we have [6]

$$M_1(G) = Z'(G;1) \tag{4}$$

$$\mathrm{M}_{\min}(G) = \left[\frac{\partial}{\partial x} M(G;x,y)\right]_{x=y=1} \tag{5}$$

$$\mathrm{M}_{\max}(G) = \left[\frac{\partial}{\partial y} M(G;x,y)\right]_{x=y=1} \tag{6}$$

$$M_2(G) = \left[\frac{\partial^2}{\partial x \partial y} M(G;x,y)\right]_{x=y=1} \tag{7}$$

$$M_3(G) = \left[\frac{\partial}{\partial y} M(G;x,y) - \frac{\partial}{\partial x} M(G;x,y)\right]_{x=y=1} \tag{8}$$

$$r(G) = \left[\frac{\partial}{\partial q} \left[\Theta_x \Theta_y M(G;x,y)\right]_{x=y=q}\right]_{q=1} \tag{9}$$

where $\Theta_t = t\frac{\partial}{\partial t}$. Moreover, if G is connected and is not a single isolated vertex, then we have

$$\mathrm{SSD}(G) = \int_0^1 \frac{\left[\Theta_x Z(G;x,y)\right]_{x=1}}{y}\, \mathrm{d}y \tag{10}$$

$$h(G) = 2\int_0^1 \frac{Z(G;q)}{q}\,\mathrm{d}q \tag{11}$$

$$I(G) = \int_0^1 \frac{\left[\Theta_x\Theta_y M(G;x,y)\right]_{x=y=q}}{q}\,\mathrm{d}q\,. \tag{12}$$

Finally, the *degree polynomial* of G is defined by

$$D(G;q) = \sum_{v\in V(G)} q^{d(v)}\,.$$

In this paper, we will determine all these indices for the connected *antiregular graphs* [1, 31–33, 35] (also called *maximally nonregular graphs* [56], or *quasiperfect graphs* [4, 37, 42]). Since in any graph of order at least two there are at least two vertices with the same degree, an antiregular graph is a graph with at most two vertices with the same degree. For any $n \in \mathbb{N}$, $n \geq 2$, there exists only one connected antiregular graph A_n on n vertices and there exists only one non-connected antiregular graph on n vertices (given by the complementary graph $\overline{A}_n$). The antiregular graph A_n can be described in several ways. Here, we consider A_n as the graph with vertex set $[n] = \{1,2,\ldots,n\}$, where two vertices $i, j \in [n]$ are adjacent whenever $i + j \geq n+1$. See Figure 1 for some examples. Notice that A_n contains exactly two vertices of the same degree (for $n \geq 2$).

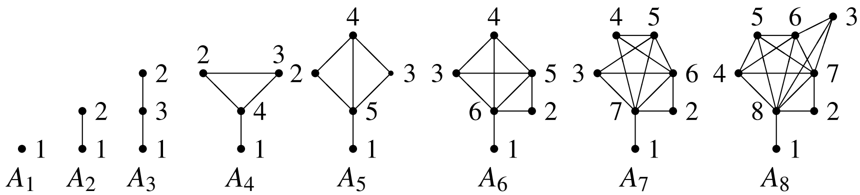

Figure 1: The first connected antiregular graphs A_n.

The antiregular graphs can also be defined recursively [35]. Recall that the *sum* of two graphs G_1 and G_2 is the graph $G_1 + G_2$ obtained by the disjoint union of the two graphs, and that the *complete sum* of G_1 and G_2 is the graph $G_1 \boxplus G_2$ obtained by $G_1 + G_2$ joining every vertex of G_1 to every vertex of G_2. Then, the connected antiregular graphs are defined by the recurrence

$$A_{n+2} = K_1 \boxplus (K_1 + A_n) \tag{13}$$

with the initial conditions $A_0 = K_0$ and $A_1 = K_1$, where K_n denotes the complete graph on n vertices. Notice that, for simplicity, we start from the empty graph A_0, even if it is not connected. See Figure 2 for a schematic representation of this recurrence.

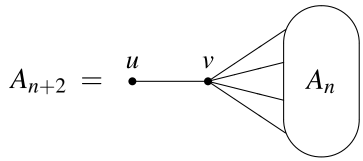

Figure 2: Recurrent structure of the connected antiregular graphs, where $u = 1$ and $v = n+2$. In particular $d_{n+2}(u) = 1$ and $d_{n+2}(v) = n+1$.

The number of edges of A_n is given by

$$\ell_n = \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil = \left\lfloor \frac{n^2}{4} \right\rfloor = \frac{2n^2 - 1 + (-1)^n}{8} . \tag{14}$$

These numbers form sequence A002620 in [45], and have generating series

$$\ell(t) = \sum_{n \geq 0} \ell_n t^n = \frac{t^2}{(1-t)^3(1+t)} . \tag{15}$$

The degree of a vertex i in A_n is

$$d_n(i) = \begin{cases} i & \text{if } i \leq \lfloor \frac{n}{2} \rfloor \\ i-1 & \text{if } i \geq \lfloor \frac{n}{2} \rfloor + 1 \end{cases}$$

while the distance between two vertices i and j in A_n is

$$d_n(i,j) = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } i \neq j ,\ i+j \geq n+1 \\ 2 & \text{if } i \neq j ,\ i+j \leq n . \end{cases}$$

Remark 1.1. Consider A_{n+2} and its decomposition described in Figure 2. Then, we have $d_{n+2}(w) = d_n(w) + 1$ and $d_{n+2}(w_1, w_2) = d_n(w_1, w_2)$ for all vertices w, w_1 and w_2 belonging to the subgraph isomorphic with A_n. These simple remark will be used several times in the rest of the paper.

Remark 1.2. To obtain some of the mentioned descriptors, we will use some elementary techniques from the theory of formal series (see [19, 41] for a classical introduction). In particular, we will often use the identity

$$\sum_{n \geq 0} \binom{n-r+s}{s} t^n = \frac{t^r}{(1-t)^{s+1}} \qquad (r, s \in \mathbb{N}) .$$

2. Wiener indices

The k-Wiener indices can be determined directly in a very simple way, as shown in the next theorem.

Theorem 2.1. *The k-Wiener indices of the antiregular graphs A_n are*

$$\mathcal{W}_k(A_n) = 2^k \binom{n}{2} - (2^k - 1) \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil . \tag{16}$$

In particular, the Wiener, the hyper-Wiener and the Harary indices are

$$\begin{aligned} \mathcal{W}(A_n) &= n^2 - n - \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil \\ \mathcal{WW}(A_n) &= 3\binom{n}{2} - 2\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil \\ \mathcal{H}(A_n) &= \frac{1}{2}\binom{n}{2} + \frac{1}{2}\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil . \end{aligned}$$

Proof. Let i and j be two distinct vertices of A_n. Since $d_n(i,j) = 1$ when i and j are adjacent and $d_n(i,j) = 2$ when i and j are not adjacent, we have at once

$$\mathcal{W}_k(A_n) = \ell_n + 2^k \left(\binom{n}{2} - \ell_n \right) = 2^k \binom{n}{2} - (2^k - 1)\ell_n$$

which simplifies in (16). □

The first values of the Winer index $\mathcal{W}(A_n)$ are: 0, 0, 1, 4, 8, 14, 21, 30, 40, 52, 65, 80, 96, 114, 133 (sequence A006578 in [45]). The first values of the hyper-Winer index $\mathcal{WW}(A_n)$ are: 0, 0, 1, 5, 10, 18, 27, 39, 52, 68, 85, 105, 126, 150, 175 (sequence A035608 in [45]). The first values of the Harary index $\mathcal{H}(A_n)$ are: 0, 0, 0, 1/2, 1, 2, 3, 9/2, 6, 8, 10, 25/2, 15, 18, 21, 49/2, 28, 32, 36, 81/2, 45, 50, 55, 121/2, 66, 72, 78, 169/2.

Notice that the recurrent structure of the antiregular graphs (described in Figure 2) implies a simple recurrence for the Wiener indices. This approach will be used very often, in the sequel.

Theorem 2.2. *The k-Wiener indices $w_n^{(k)} = \mathcal{W}_k(A_n)$ satisfy the linear recurrence*

$$w_{n+2}^{(k)} = w_n^{(k)} + (2^k + 1)n + 1 \tag{17}$$

with the initial values $w_0^{(k)} = w_1^{(k)} = 0$.

Proof. Consider A_{n+2} and the decomposition in Figure 2. Then, we have

$$w_n^{(k)} = d_{n+2}(u,v)^k + \sum_{w \in V(A_n)} d_{n+2}(u,w)^k + \sum_{w \in V(A_n)} d_{n+2}(v,w)^k + \sum_{w_1,w_2 \in V(A_n)} d_{n+2}(w_1,w_2).$$

Now, by Remark 1.1, we have

$$w_{n+2}^{(k)} = 1 + 2^k n + n + \sum_{w_1,w_2 \in V(A_n)} d_n(w_1,w_2) = 1 + 2^k n + n + w_n^{(k)}.$$

This is recurrence (17). □

In the sequel, we will need the following result.

Theorem 2.3. *The generating series for the k-Wiener indices of the antiregular graphs A_n is*

$$W_k(t) = \sum_{n \geq 0} \mathcal{W}_k(A_n)\, t^n = \frac{t^2 + 2^k t^3}{(1-t)^3(1+t)}. \tag{18}$$

In particular, the generating series for the Wiener indices is

$$w(t) = \sum_{n \geq 0} \mathcal{W}(A_n)\, t^n = \frac{t^2 + 2t^3}{(1-t)^3(1+t)}. \tag{19}$$

Proof. By formula (16) and series (15), we have

$$\sum_{n \geq 0} \mathcal{W}_k(A_n)\, t^n = 2^k \sum_{n \geq 0} \binom{n}{2} t^n - (2^k - 1)\ell(t) = \frac{2^k t^2}{(1-t)^3} - \frac{(2^k-1)t^2}{(1-t)^3(1+t)}$$

which simplifies in series (18). Equivalently, this series can be obtained by the recurrence and the initial values stated in Theorem 2.2. □

3. Degree distance

In this case, we start by obtaining a recurrence for the degree distances.

Theorem 3.1. *The degree distances $d_n = \mathcal{D}(A_n)$ satisfy the recurrence*

$$d_{n+2} = d_n + n^2 + 7n + 2 + 6\ell_n + 2w_n \tag{20}$$

with the initial values $d_0 = d_1 = 0$.

Proof. Consider A_{n+2} and the decomposition in Figure 2. By Remark 1.1, we have

$$\begin{aligned}
d_{n+2} &= (d_{n+2}(u) + d_{n+2}(v))\, d_{n+2}(u,v) \\
&\quad + \sum_{w \in V(A_n)} (d_{n+2}(u) + d_{n+2}(w))\, d_{n+2}(u,w) \\
&\quad + \sum_{w \in V(A_n)} (d_{n+2}(v) + d_{n+2}(w))\, d_{n+2}(v,w) \\
&\quad + \sum_{\{w_1,w_2\} \subseteq V(A_n)} (d_{n+2}(w_1) + d_{n+2}(w_2))\, d_{n+2}(w_1,w_2) \\
&= n+2+2 \sum_{w \in V(A_n)} (2 + d_n(w)) + \sum_{w \in V(A_n)} (n+2+d_n(w)) \\
&\quad + \sum_{\{w_1,w_2\} \subseteq V(A_n)} (2 + d_n(w_1) + d_n(w_2))\, d_n(w_1,w_2) \\
&= n+2+4n+4\ell_n + (n+2)n + 2\ell_n + 2w_n + d_n \\
&= n^2 + 7n + 2 + 6\ell_n + 2w_n + d_n\,.
\end{aligned}$$

This is recurrence (20). □

Now, by using the previous result, we can obtain the generating series for the degree distances.

Theorem 3.2. *The generating series for the degree distances d_n is*

$$d(t) = \sum_{n \geq 0} d_n t^n = \frac{2t^2(1+3t+4t^2)}{(1-t)^4(1+t)^2}\,. \tag{21}$$

Proof. By recurrence (20), with the relative initial values, we obtain at once the equation

$$\frac{d(t)}{t^2} = d(t) + \sum_{n \geq 0} (n^2 + 7n + 2)t^n + 6\ell(t) + 2w(t)$$

or

$$d(t) = t^2 d(t) + \frac{2t^2(1+2t-2t^2)}{(1-t)^3} + 6t^2\ell(t) + 2t^2 w(t)$$

from which we have

$$d(t) = \frac{2t^2(1+2t-2t^2)}{(1-t^2)(1-t)^3} + \frac{6t^2}{1-t^2}\,\ell(t) + \frac{2t^2}{1-t^2}\,w(t)\,.$$

By series (15) and (19), we obtain series (21). □

Finally, by their generating series, we can derive an explicit expression for the degree distances.

Theorem 3.3. *The degree distance of the antiregular graph A_n is*

$$\mathcal{D}(A_n) = \frac{16n^3 - 18n^2 - 10n + 9}{24} + (-1)^n \frac{2n-3}{8}. \tag{22}$$

Proof. Series (21) admits the following decomposition in partial fractions:

$$d(t) = \frac{4}{(1-t)^4} - \frac{19}{2}\frac{1}{(1-t)^3} + \frac{13}{2}\frac{1}{(1-t)^2} - \frac{5}{8}\frac{1}{1-t} + \frac{1}{4}\frac{1}{(1+t)^2} - \frac{5}{8}\frac{1}{1+t}.$$

Hence, extracting the coefficient of t^n, we have the identity

$$d_n = 4\binom{n+3}{3} - \frac{19}{2}\binom{n+2}{2} + \frac{13}{2}\binom{n+1}{1} - \frac{5}{8} + (-1)^n \frac{1}{4}\binom{n+1}{1} - (-1)^n \frac{5}{8}$$

which simplifies in (22). □

4. Gutman index

Also in this case, we start by determining a recurrence for the Gutman indices. Then, from this recurrence, we obtain their generating series, and, finally, by expanding this series, we obtain an explicit formula for these indices.

Theorem 4.1. *The Gutman indices $g_n = \mathrm{Gut}(A_n)$ satisfy the recurrence*

$$g_{n+2} = g_n + d_n + w_n + 2(n+3)\ell_n + n^2 + 4n + 1 \tag{23}$$

with the initial values $g_0 = g_1 = 0$.

Proof. Consider A_{n+2}. By the decomposition described in Figure 2 and by Remark 1.1, we have

$$\begin{aligned}
g_{n+2} &= d_{n+2}(u)d_{n+2}(v)\,d_{n+2}(u,v) \\
&\quad + \sum_{w\in V(A_n)} d_{n+2}(u)d_{n+2}(w)\,d_{n+2}(u,w) \\
&\quad + \sum_{w\in V(A_n)} d_{n+2}(v)d_{n+2}(w)\,d_{n+2}(v,w) \\
&\quad + \sum_{\{w_1,w_2\}\subseteq V(A_n)} d_{n+2}(w_1)d_{n+2}(w_2)\,d_{n+2}(w_1,w_2) \\
&= n+1+2\sum_{w\in V(A_n)}(d_n(w)+1) + (n+1)\sum_{w\in V(A_n)}(d_n(w)+1) \\
&\quad + \sum_{\{w_1,w_2\}\subseteq V(A_n)} (d_n(w_1)+1)(d_n(w_2)+1)\,d_n(w_1,w_2) \\
&= n+1+2(2\ell_n+n)+(n+1)(2\ell_n+n)
\end{aligned}$$

$$+ \sum_{\{w_1,w_2\}\subseteq V(A_n)} (d_n(w_1)d_n(w_2)+d_n(w_1)+d_n(w_2)+1)\, d_n(w_1,w_2)$$
$$= n^2+4n+1+2(n+3)\ell_n+g_n+d_n+w_n\,.$$

This is recurrence (23). □

Theorem 4.2. *The generating series for the Gutman indices is*

$$g(t) = \sum_{n\geq 0} g_n t^n = \frac{t^2(1+4t+13t^2+6t^3+4t^4)}{(1-t)^5(1+t)^3}\,. \tag{24}$$

Proof. By recurrence (23), with the relative initial values, we immediately have the equation

$$\frac{g(t)}{t^2} = g(t)+d(t)+w(t)+2\sum_{n\geq 0}(n+3)\ell_n t^n + \sum_{n\geq 0}(n^2+4n+1)t^n$$

or

$$g(t) = t^2 g(t)+t^2 d(t)+t^2 w(t)+2t^2\sum_{n\geq 0}(n+3)\ell_n t^n + t^2\sum_{n\geq 0}(n^2+4n+1)t^n$$

from which we have

$$g(t) = \frac{t^2}{1-t^2}\, d(t) + \frac{t^2}{1-t^2}\, w(t) + \frac{2t^2}{1-t^2}\,(t\ell'(t)+3\ell(t)) + \frac{t^2}{1-t^2}\frac{1+3t-2t^2}{(1-t)^3}\,.$$

Using series (21), (19) and (15) and simplifying, we obtain series (24). □

Theorem 4.3. *The Gutman index of the antiregular graph A_n is*

$$\mathrm{Gut}(A_n) = \frac{14n^4-16n^3-8n^2+4n+3}{96} + (-1)^n\frac{4n^2-4n-1}{32}\,. \tag{25}$$

Proof. Series (24) admits the following decomposition in partial fractions:

$$g(t) = \frac{7}{2}\frac{1}{(1-t)^5} - \frac{39}{4}\frac{1}{(1-t)^4} + \frac{73}{8}\frac{1}{(1-t)^3} - \frac{49}{16}\frac{1}{(1-t)^2} + \frac{7}{32}\frac{1}{1-t}$$
$$+ \frac{1}{4}\frac{1}{(1+t)^3} - \frac{1}{2}\frac{1}{(1+t)^2} + \frac{7}{32}\frac{1}{1+t}\,.$$

Hence, extracting the coefficient of t^n, we have the identity

$$g_n = \frac{7}{2}\binom{n+4}{4} - \frac{39}{4}\binom{n+3}{3} + \frac{73}{8}\binom{n+2}{2} - \frac{49}{16}\binom{n+1}{1} + \frac{7}{32}$$
$$+(-1)^n\frac{1}{4}\binom{n+2}{2} - (-1)^n\frac{1}{2}\binom{n+1}{1} + (-1)^n\frac{7}{32}$$

which simplifies in (25). □

The first values of the Gutman index g_n are: 0, 1, 6, 27, 66, 154, 284, 514, 820, 1295, 1890, 2741, 3766, 5152, 6776, 8884, 11304, 14349.

5. Zagreb indices

The first Zagreb index can be obtained directly in the following simple way.

Theorem 5.1. *The first Zagreb index of the antiregular graph A_n is*

$$M_1(A_n) = \frac{n(n-1)(2n-1)}{6} + \left\lfloor \frac{n}{2} \right\rfloor^2 . \tag{26}$$

Proof. The degree sequence of A_n is $\big(1,2,\ldots,\lfloor\frac{n}{2}\rfloor,\lfloor\frac{n}{2}\rfloor,\ldots,n-1\big)$, where $\lfloor\frac{n}{2}\rfloor$ is the only element repeated twice. Therefore, we have

$$M_1(A_n) = \sum_{k=1}^{n-1} k^2 + \left\lfloor \frac{n}{2} \right\rfloor^2$$

which simplifies in (26). □

Remark 5.2. Also the indices $m_n = M_1(A_n)$ satisfy a recurrence. Indeed, by using the decomposition of A_{n+2} (see Figure 2) and Remark 1.1, we have

$$\begin{aligned} m_{n+2} &= d_{n+2}(u)^2 + d_{n+2}(v)^2 + \sum_{w\in V(A_n)} d_{n+2}(w)^2 \\ &= 1 + (n+1)^2 + \sum_{w\in V(A_n)} (d_n(w)+1)^2 \\ &= n^2+2n+2+\sum_{w\in V(A_n)} (d_n(w)^2+2d_n(w)+1) \\ &= n^2+2n+2+m_n+4\ell_n+n \end{aligned}$$

that is

$$m_{n+2} = m_n + 4\ell_n + n^2 + 3n + 2 .$$

Now, let $m(t) = \sum_{n\geq 0} m_n t^n$ be the generating series for the indices m_n. Then, by the above recurrence with the initial values $m_0 = m_1 = 0$, we have at once the equation

$$\frac{m(t)}{t^2} = m(t) + 4\ell(t) + \sum_{n\geq 0} (n^2+3n+2)t^n$$

that is

$$m(t) = t^2 m(t) + 4t^2\ell(t) + \frac{2t^2}{(1-t)^3}$$

or

$$m(t) = \frac{4t^2}{1-t^2}\,\ell(t) + \frac{2t^2}{(1-t^2)(1-t)^3} .$$

Finally, by series (15), we obtain the generating series

$$m(t) = \sum_{n\geq 0} m_n t^n = \frac{2(t^2+t^3+2t^4)}{(1-t)^4(1+t)^2} \tag{27}$$

For the second Zagreb index, we proceed by first obtaining a recurrence, then their generating series and, finally, an explicit formula.

Theorem 5.3. *The second Zagreb indices $M_n = M_2(A_n)$ satisfy the recurrence*

$$M_{n+2} = M_n + m_n + (2n+3)\ell_n + (n+1)^2 \tag{28}$$

with the initial values $M_0 = M_1 = 0$.

Proof. Consider A_{n+2} and its decomposition in Figure 2. By Remark 1.1, we have

$$\begin{aligned}
M_{n+2} &= d_{n+2}(u)d_{n+2}(v) + \sum_{w\in V(A_n)} d_{n+2}(v)d_{n+2}(w) \\
&\quad + \sum_{\{w_1,w_2\}\in E(A_n)} d_{n+2}(w_1)d_{n+2}(w_2) \\
&= n+1+(n+1)\sum_{w\in V(A_n)} (d_n(w)+1) \\
&\quad + \sum_{\{w_1,w_2\}\in E(A_n)} (d_n(w_1)+1)(d_n(w_2)+1) \\
&= n+1+(n+1)(2\ell_n+n) \\
&\quad + \sum_{\{w_1,w_2\}\in E(A_n)} (d_n(w_1)d_n(w_2)+d_n(w_1)+d_n(w_2)+1) \\
&= (n+1)(2\ell_n+n+1)+M_n+m_n+\ell_n \\
&= (2n+3)\ell_n+(n+1)^2+M_n+m_n\,.
\end{aligned}$$

This is recurrence (28). □

Theorem 5.4. *The generating series for the second Zagreb indices of the connected antiregular graphs is*

$$M(t) = \sum_{n\geq 0} M_n t^n = \frac{t^2(1+2t+9t^2+4t^3+4t^4)}{(1-t)^5(1+t)^3}\,. \tag{29}$$

Proof. By recurrence (28) and the relative initial values, we obtain the equation

$$\frac{M(t)}{t^2} = M(t)+m(t)+\sum_{n\geq 0}(2n+3)\ell_n t^n + \sum_{n\geq 0}(n+1)^2 t^n$$

that is

$$M(t) = t^2M(t)+t^2m(t)+t^2(2t\ell'(t)+3\ell(t)) + \frac{t^2(1+t)}{(1-t)^3}$$

from which we have

$$M(t)=\frac{t^2}{1-t^2}\,m(t)+\frac{t^2}{1-t^2}\,(2t\ell'(t)+3\ell(t))+\frac{t^2(1+t)}{(1-t^2)(1-t)^3}\,.$$

Replacing series (27) and (15), we obtain series (29). □

Theorem 5.5. *The second Zagreb index of the antiregular graph A_n is*

$$M_2(A_n)=\frac{10n^4-16n^3+8n^2+4n-3}{96}+(-1)^n\,\frac{(2n-1)^2}{32}\,. \tag{30}$$

Proof. Series (29) admits the following decomposition in partial fractions:

$$\begin{aligned}M(t)=\frac{5}{2}\,\frac{1}{(1-t)^5}-\frac{29}{4}\,\frac{1}{(1-t)^4}+\frac{59}{8}\,\frac{1}{(1-t)^3}-\frac{47}{16}\,\frac{1}{(1-t)^2}+\frac{9}{32}\,\frac{1}{1-t}\\+\frac{1}{4}\,\frac{1}{(1+t)^3}-\frac{1}{2}\,\frac{1}{(1+t)^2}+\frac{9}{32}\,\frac{1}{1+t}\,.\end{aligned}$$

Then, we have the identity

$$\begin{aligned}M_n=\frac{5}{2}\binom{n+4}{4}-\frac{29}{4}\binom{n+3}{3}+\frac{59}{8}\binom{n+2}{2}-\frac{47}{16}\binom{n+1}{1}+\frac{9}{32}\\+(-1)^n\frac{1}{4}\binom{n+2}{2}-(-1)^n\frac{1}{2}\binom{n+1}{1}+(-1)^n\frac{9}{32}\end{aligned}$$

which simplifies in (30). □

For the third Zagreb index, we proceed, as before, by obtaining a recurrence, the generating series and, finally, an explicit formula.

Theorem 5.6. *The third Zagreb indices $\mu_n=M_3(A_n)$ satisfy the recurrence*

$$\mu_{n+2}=\mu_n-2\ell_n+n^2+n \tag{31}$$

with the initial values $\mu_0=\mu_1=0$.

Proof. Consider A_{n+2} and its decomposition in Figure 2. Then, by Remark 1.1, we have

$$\begin{aligned}\mu_{n+2}&=|d_{n+2}(u)-d_{n+2}(v)|+\sum_{w\in V(A_n)}|d_{n+2}(v)-d_{n+2}(w)|\\&\quad+\sum_{\{w_1,w_2\}\in E(A_n)}|d_{n+2}(w_1)-d_{n+2}(w_2)|\\&=n+\sum_{w\in V(A_n)}(n-d_n(w))+\sum_{\{w_1,w_2\}\in E(A_n)}|d_n(w_1)-d_n(w_2)|\\&=n+n^2-2\ell_n+\mu_n\,.\end{aligned}$$

This is recurrence (31). □

Theorem 5.7. *The generating series for the third Zagreb indices of the connected antiregular graphs is*

$$\mu(t) = \sum_{n\geq 0} \mu_n t^n = \frac{2t^3}{(1-t)^4(1+t)^2}\,. \tag{32}$$

Proof. By recurrence (31) and the relative initial values, we obtain the equation

$$\frac{\mu(t)}{t^2} = \mu(t) - 2\ell(t) + \frac{2t}{(1-t)^3}$$

that is

$$\mu(t) = t^2\mu(t) - 2t^2\ell(t) + \frac{2t^3}{(1-t)^3}$$

from which we have

$$\mu(t) = \frac{2t^3}{(1-t^2)(1-t)^3} - \frac{2t^2}{1-t^2}\,\ell(t)\,.$$

Replacing series (15), we obtain series (32). □

Theorem 5.8. *The third Zagreb index of the antiregular graph A_n is*

$$M_3(A_n) = \frac{2n^3-5n}{24} - (-1)^n\,\frac{n}{8}\,. \tag{33}$$

Proof. Series (32) admits the following decomposition in partial fractions:

$$\mu(t) = \frac{1}{2}\,\frac{1}{(1-t)^4} - \frac{1}{(1-t)^3} + \frac{3}{8}\,\frac{1}{(1-t)^2} - \frac{1}{8}\,\frac{1}{1-t} - \frac{1}{8}\,\frac{1}{(1+t)^2} + \frac{1}{8}\,\frac{1}{1+t}\,.$$

Then, we have the identity

$$\mu_n = \frac{1}{2}\binom{n+3}{3} - \binom{n+2}{2} + \frac{3}{8}\binom{n+1}{1} - \frac{1}{8} - (-1)^n\frac{1}{8}\binom{n+1}{1} + (-1)^n\frac{1}{8}$$

which simplifies in (33). □

Now, using the previous results, we can deduce very easily the reduced Zagreb indices, the Bell index (and the variance of the vertex degrees), the forgotten Zagreb index and the hyper-Zagreb index.

Theorem 5.9. *The reduced Zagreb indices of the antiregular graph A_n are*

$$\mathrm{RM}_1(A_n) = \frac{8n^3-30n^2+22n+15}{24} + (-1)^n\frac{2n-5}{8} \tag{34}$$

$$\mathrm{RM}_2(A_n) = \frac{10n^4-48n^3+56n^2+12n-27}{96} + (-1)^n\frac{(3-2n)^2}{32}\,. \tag{35}$$

Proof. For the reduced Zagreb indices we have $\mathrm{RM}_1(A_n) = M_1(A_n) + n - 4\ell_n$ and $\mathrm{RM}_2(A_n) = M_2(A_n) - M_1(A_n) + \ell_n$. By formulas (30), (26), (14) and identity $\lfloor \frac{n}{2} \rfloor = \frac{2n-1+(-1)^n}{4}$, we can deduce straightforwardly the stated formulas. □

Theorem 5.10. *The Bell index of the antiregular graph A_n is*

$$B(A_n) = \frac{n(n-1)(2n-1)}{6} + \left\lfloor \frac{n}{2} \right\rfloor^2 \left(1 - \frac{4}{n} \left\lceil \frac{n}{2} \right\rceil^2\right) \qquad (n \geq 1). \tag{36}$$

Proof. Immediate consequence of the definition of the Bell index and of identity (26). □

Theorem 5.11. *The forgotten Zagreb index of the antiregular graph A_n is*

$$F(A_n) = \frac{n^2(n-1)^2}{4} + \left\lfloor \frac{n}{2} \right\rfloor^3. \tag{37}$$

Proof. Since the degree sequence of A_n is $\big(1, 2, \ldots, \lfloor \frac{n}{2} \rfloor, \lfloor \frac{n}{2} \rfloor, \ldots, n-1\big)$, we have

$$F(A_n) = \sum_{k=1}^{n-1} k^3 + \left\lfloor \frac{n}{2} \right\rfloor^3$$

which simplifies in (37). □

Theorem 5.12. *The hyper-Zagreb index of the antiregular graph A_n is*

$$HM(A_n) = \frac{22n^4 - 40n^3 + 20n^2 + 4n - 3}{48} + \left\lfloor \frac{n}{2} \right\rfloor^3 + (-1)^n \frac{(2n-1)^2}{16}. \tag{38}$$

Proof. Since $HM(A_n) = F(A_n) + 2M_2(A_n)$, by identities (37) and (30), we have

$$\begin{aligned} HM(A_n) = {} & \frac{n^2(n-1)^2}{4} + \left\lfloor \frac{n}{2} \right\rfloor^3 \\ & + \frac{10n^4 - 16n^3 + 8n^2 + 4n - 3}{48} + (-1)^n \frac{(2n-1)^2}{16}. \end{aligned}$$

By simplifying, we obtain identity (38). □

The first values of these indices are listed in the following table.

n	0	1	2	3	4	5	6	7	8	9	10	11	12
$M_1(A_n)$	0	0	2	6	18	34	64	100	156	220	310	410	542
$M_2(A_n)$	0	0	1	4	19	44	106	192	354	560	895	1300	1901
$M_3(A_n)$	0	0	0	2	4	10	16	28	40	60	80	110	140
$\mathrm{RM}_1(A_n)$	0	1	0	1	6	15	34	59	100	149	220	301	410
$\mathrm{RM}_2(A_n)$	0	0	0	0	5	16	51	104	214	360	610	920	1395
$B(A_n)$	0	0	0	$\frac{2}{3}$	2	$\frac{26}{5}$	10	$\frac{124}{7}$	28	$\frac{380}{9}$	60	$\frac{910}{11}$	110
$F(A_n)$	0	0	2	10	44	108	252	468	848	1360	2150	3150	4572
$HM(A_n)$	0	0	4	18	82	196	464	852	1556	2480	3940	5750	8374

6. Zagreb polynomials

For the Zagreb polynomials we obtain a recurrence and then their generating series. First, however, we need the following result.

Lemma 6.1. *The generating series of the degree polynomials $D_n(q) = D(A_n;q)$ of the connected antiregular graphs is*

$$D(q;t) = \sum_{n\geq 0} D_n(q)t^n = \frac{t-(1-q)t^2-q^2t^3}{(1-t)(1-qt)(1-qt^2)}\,. \tag{39}$$

Proof. Since the degree sequence of A_n is $\left(1,2,\ldots,\lfloor\frac{n}{2}\rfloor,\lfloor\frac{n}{2}\rfloor,\ldots,n-1\right)$, we have

$$D_n(q) = \sum_{k=1}^{n-1} q^k + q^{\lfloor n/2\rfloor} = \frac{1-q^n}{1-q} - 1 + q^{\lfloor n/2\rfloor}\,.$$

Consequently, we have the generating series

$$D(q;t) = \frac{1}{1-q}\left(\frac{1}{1-t}-\frac{1}{1-qt}\right) - \frac{1}{1-t} + \frac{1+t}{1-qt^2}$$

which simplifies in series (39). □

Theorem 6.2. *The M-polynomials $M_n(x,y) = M(A_n;x,y)$ of the connected antiregular graphs satisfy the recurrence*

$$M_{n+2}(x,y) = xyM_n(x,y) + xy^{n+1}D_n(x) + xy^{n+1} \tag{40}$$

with the initial values $M_0(x,y) = M_1(x,y) = 0$.

In particular, the Zagreb polynomials $Z_n(q) = Z(A_n;q)$ satisfy the recurrence

$$Z_{n+2}(q) = q^2Z_n(q) + q^{n+2}D_n(q) + q^{n+2} \tag{41}$$

with the initial values $Z_0(q) = Z_1(q) = 0$.

Proof. Consider A_{n+2} and its decomposition in Figure 2. By Remark 1.1, we have

$$\begin{aligned} M_{n+2}(x,y) &= x^{\min(d_{n+2}(u),d_{n+2}(v))}y^{\max(d_{n+2}(u),d_{n+2}(v))} \\ &\quad + \sum_{w\in V(A_n)} x^{\min(d_{n+2}(v),d_{n+2}(w))}y^{\max(d_{n+2}(v),d_{n+2}(w))} \\ &\quad + \sum_{\{w_1,w_2\}\in E(A_n)} x^{\min(d_{n+2}(w_1),d_{n+2}(w_2))}y^{\max(d_{n+2}(w_2),d_{n+2}(w_1))} \\ &= xy^{n+1} + \sum_{w\in V(A_n)} x^{d_n(w)+1}y^{n+1} \end{aligned}$$

$$+\sum_{\{w_1,w_2\}\in E(A_n)} x^{\min(d_n(w_1),d_n(w_2))+1}y^{\max(d_n(w_2),d_n(w_1))+1}$$
$$= xy^{n+1}+xy^{n+1}D_n(x)+xyM_n(x,y)\,.$$

This is recurrence (40). Recurrence (41) can be obtain with a similar argument, or by setting $x=y=q$ and using formula (3). □

Theorem 6.3. *The generating series for the M-polynomials is*

$$M(x,y;t)=\sum_{n\geq 0}M_n(x,y)\,t^n=\frac{xyt^2(1+(1-x)yt-y^2t^2)}{(1-yt)(1-xyt)(1-xyt^2)(1-xy^2t^2)}\,. \tag{42}$$

In particular, the generating series for the Zagreb polynomials is

$$Z(q;t)=\sum_{n\geq 0}Z_n(q)\,t^n=\frac{q^2t^2(1+(q-q^2)t-q^2t^2)}{(1+qt)(1-qt)^2(1-q^2t)(1-q^3t^2)}\,. \tag{43}$$

Proof. By recurrence (40) and its initial values, we have the equation

$$\frac{M(x,y;t)}{t^2}=xyM(x,y;t)+xD(x;yt)+\frac{xy}{1-yt}$$

from which we have

$$M(x,y;t)=\frac{xyt^2}{1-xyt^2}\,D(x;yt)+\frac{xyt^2}{(1-yt)(1-xyt^2)}\,.$$

By replacing series (39), we obtain series (42). Series (43) can be obtained from recurrence (40), or by setting $x=y=q$ and using formula (3). □

Remark 6.4. In a similar way, we can prove that the symmetric Zagreb polynomials $Z_n(x,y)=Z(A_n;x,y)$ satisfy the recurrence

$$Z_{n+2}(x,y)=xyZ_n(x,y)+xy^{n+1}D_n(x)+x^{n+1}yD_n(y)+xy(x^n+y^n) \tag{44}$$

with the initial values $Z_0(x,y)=Z_1(x,y)=0$, and that their generating series $Z(x,y;t)=\sum_{n\geq 0}Z_n(x,y)\,t^n$ is

$$Z(x,y;t)=\frac{xyt^2N(x,y;t)}{(1-xt)(1-yt)(1-xyt)(1-xyt^2)(1-x^2yt^2)(1-xy^2t^2)} \tag{45}$$

where $N(x,y;t)=2-2xyt-(x+y)^2t^2+xy(xy(x+y)+(x-y)^2+x+y)t^3-x^2y^2(x^2+y^2-2x-2y)t^4-2x^3y^3t^5$.

All the distance-based indices can be obtained, or reobtained, by using series (42). For instance, we have the following results.

Theorem 6.5. *The min-deg and the max-deg indices of the antiregular graph A_n are*

$$\mathrm{M}_{\min}(A_n) = \frac{1}{16}(2n^3 - 2n^2 + n + 1 + (-1)^n(3n-1)) \tag{46}$$
$$\mathrm{M}_{\max}(A_n) = \frac{1}{48}\,(n-1)(10n^2 + 4n - 3 + (-1)^n 3)\,. \tag{47}$$

Proof. By formulas (5) and (6) and by series (42), we have

$$\begin{aligned}
\sum_{n\geq 0} \mathrm{M}_{\min}(A_n)\,t^n &= \frac{t^2+2t^4}{(1-t)^4(1+t)^2} \\
&= \frac{3}{4}\frac{1}{(1-t)^4} - \frac{7}{4}\frac{1}{(1-t)^3} + \frac{21}{16}\frac{1}{(1-t)^2} - \frac{1}{4}\frac{1}{1-t} + \frac{3}{16}\frac{1}{(1+t)^2} - \frac{1}{4}\frac{1}{1+t} \\
\sum_{n\geq 0} \mathrm{M}_{\max}(A_n)\,t^n &= \frac{t^2+2t^3+2t^4}{(1-t)^4(1+t)^2} \\
&= \frac{5}{4}\frac{1}{(1-t)^4} - \frac{11}{4}\frac{1}{(1-t)^3} + \frac{27}{16}\frac{1}{(1-t)^2} - \frac{1}{8}\frac{1}{1-t} + \frac{1}{16}\frac{1}{(1+t)^2} - \frac{1}{8}\frac{1}{1+t}\,.
\end{aligned}$$

Expanding this series we obtain formulas (46) and (47). □

Theorem 6.6. *The refined Zagreb index of the antiregular graph A_n is*

$$\begin{aligned}
r(A_n) = {} & \frac{288n^5 - 710n^4 + 620n^3 + 50n^2 - 248n + 45}{1920} \\
& + (-1)^n \frac{76n^3 - 114n^2 + 56n - 9}{384}\,.
\end{aligned} \tag{48}$$

Proof. Using formula (9) and series (42), it is straightforward to obtain the generating series

$$r(t) = \sum_{n\geq 0} r(A_n)\,t^n = \frac{2t^2(1+4t+29t^2+32t^3+53t^4+17t^5+8t^6)}{(1-t)^6(1+t)^4}\,.$$

Then, by decomposing this series in partial fraction, we have

$$\begin{aligned}
r(t) = {} & \frac{18}{(1-t)^6} - \frac{503}{8}\frac{1}{(1-t)^5} + \frac{661}{8}\frac{1}{(1-t)^4} - \frac{789}{16}\frac{1}{(1-t)^3} + \frac{49}{4}\frac{1}{(1-t)^2} \\
& - \frac{85}{128}\frac{1}{1-t} + \frac{19}{16}\frac{1}{(1+t)^4} - \frac{95}{32}\frac{1}{(1+t)^3} + \frac{155}{64}\frac{1}{(1+t)^2} - \frac{85}{128}\frac{1}{1+t}\,.
\end{aligned}$$

Hence, we have the identity

$$r_n = 18\binom{n+5}{5} - \frac{503}{8}\binom{n+4}{4} + \frac{661}{8}\binom{n+3}{3} - \frac{789}{16}\binom{n+2}{2}$$

$$+\frac{49}{4}\binom{n+1}{1}-\frac{85}{128}+(-1)^n\frac{19}{16}\binom{n+3}{3}-(-1)^n\frac{95}{32}\binom{n+2}{2}$$
$$+(-1)^n\frac{155}{64}\binom{n+1}{1}-(-1)^n\frac{85}{128}$$

which simplifies in (48). □

Theorem 6.7. *The symmetric division index of the antiregular graph A_n is*

$$\begin{aligned}\mathrm{SSD}(A_n) &= \frac{6n^2-8n+3+(-1)^n}{8}\\ &\quad+\frac{2n-1+(-1)^n}{4}\sum_{k=1}^{n}\frac{(-1)^{k-1}}{k}+\frac{1-(-1)^n}{4n} \qquad (n\geq 1)\,.\end{aligned} \tag{49}$$

Proof. Using formula (10) and series (45), it is straightforward to obtain the generating series

$$\sum_{n\geq 0}\mathrm{SSD}(A_n)\,t^n=\frac{3t^2+3t^3-t^4+t^5}{4(1-t)^3(1+t)}+\frac{t}{4(1+t)}\ \ln\frac{1}{1-t}-\frac{t+t^2}{4(1-t)^2}\ \ln\frac{1}{1+t}\,.$$

The coefficients of the series

$$\frac{3+3t-t^2+t^3}{4(1-t)^3(1+t)}=\frac{3}{2}\frac{1}{(1-t)^3}-\frac{13}{4}\frac{1}{(1-t)^2}+\frac{19}{8}\frac{1}{1-t}-\frac{1}{8}\frac{1}{1+t}-\frac{1+t}{2}$$

are (for $n\geq 2$)

$$\frac{3}{2}\binom{n+2}{2}-\frac{13}{4}\binom{n+1}{1}+\frac{19}{8}-\frac{(-1)^n}{8}=\frac{6n^2-8n+5-(-1)^n}{8}\,.$$

The coefficients of the series $\frac{t}{1+t}\ \ln\frac{1}{1-t}$ are (for $n\geq 1$)

$$\sum_{k=1}^{n-1}\frac{(-1)^{n-k-1}}{k}=(-1)^n\sum_{k=1}^{n}\frac{(-1)^{k-1}}{k}+\frac{1}{n}$$

The coefficients of the series $\frac{t+t^2}{(1-t)^2}\ \ln\frac{1}{1+t}$ are (for $n\geq 2$)

$$\begin{aligned}&\sum_{k=1}^{n}\frac{(-1)^k}{k}(n-k)+\sum_{k=1}^{n-1}\frac{(-1)^k}{k}(n-k-1)\\ &=\sum_{k=1}^{n}\frac{(-1)^k}{k}(2n-2k-1)+\frac{(-1)^n}{n}\\ &=(2n-1)\sum_{k=1}^{n}\frac{(-1)^k}{k}-2\sum_{k=1}^{n}(-1)^k+\frac{(-1)^n}{n}\\ &=(2n-1)\sum_{k=1}^{n}\frac{(-1)^k}{k}+2\frac{1-(-1)^n}{2}+\frac{(-1)^n}{n}\,.\end{aligned}$$

Summing all these coefficients, we obtain identity (49). □

The first values of these indices are listed in the following table.

n	1	2	3	4	5	6	7	8	9	10	11	12
$\mathrm{M}_{\min}(A_n)$	0	1	2	7	12	24	36	58	80	115	150	201
$\mathrm{M}_{\max}(A_n)$	0	1	4	11	22	40	64	98	140	195	260	341
$r(A_n)$	0	2	12	88	260	790	1690	3650	6546	11796	18946	30518
$\mathrm{SSD}(A_n)$	0	2	5	$\frac{29}{3}$	$\frac{47}{3}$	$\frac{467}{20}$	$\frac{647}{20}$	$\frac{4519}{105}$	$\frac{5779}{105}$	$\frac{34639}{504}$	$\frac{42199}{504}$	$\frac{463937}{4620}$

7. Harmonic index

To determine the harmonic index of an antiregular graph we will use the Zagreb polynomials obtained in the previous section. First of all, we have

Theorem 7.1. *The harmonic index of the antiregular graph A_{n+1} is*

$$h(A_{n+1}) = 2\sum_{k=0}^{\lfloor\frac{n-1}{2}\rfloor} \frac{1}{n+k+1} + 2\sum_{k=0}^{n} \left\lfloor \frac{n-k}{2} \right\rfloor \frac{1}{n+k+1}\,. \tag{50}$$

Proof. For $n \geq 2$, the antiregular graph A_n has no isolated vertices. So, for any two adjacent vertices i and j, we have $i+j \geq n+1$ and consequently $d_n(i) + d_n(j) \geq i+j-2 \geq n-1 \geq 1$. Since $Z_0(q) = Z_1(q) = 0$, there exist polynomials $z_n(q)$ such that $Z_n(q) = q^n z_n(q)$ for every $n \in \mathbb{N}$. If $z(q;t)$ is the generating series for these polynomials, then, by identity (43), the generating series for the polynomials $z_{n+1}(q)$ is

$$\frac{z(q;t)}{t} = \frac{Z(q;t/q)}{t} = \frac{t(1+t-qt(1+t)}{(1+t)(1-t)^2(1-qt)(1-qt^2)}\,.$$

This series admits the following decomposition in partial fractions:

$$\frac{z(q;t)}{t} = \frac{t}{1-t}\,\frac{1}{1-qt^2} + \frac{t^2}{(1+t)(1-t)^2}\,\frac{1}{1-qt}\,.$$

Since [45, A004526]

$$\frac{t^2}{(1+t)(1-t)^2} = \sum_{k=0}^{n} \left\lfloor \frac{n}{2} \right\rfloor t^n\,,$$

we have

$$z_{n+1}(q) = \sum_{k=0}^{\lfloor\frac{n-1}{2}\rfloor} q^k + \sum_{k=0}^{n} \left\lfloor \frac{n-k}{2} \right\rfloor q^k$$

and

$$Z_{n+1}(q) = q^{n+1} z_{n+1}(q) = \sum_{k=0}^{\lfloor\frac{n-1}{2}\rfloor} q^{n+k+1} + \sum_{k=0}^{n} \left\lfloor \frac{n-k}{2} \right\rfloor q^{n+k+1}\,.$$

So, by formula (11), we obtain at once identity (50). $\square$

As we will prove in the next theorem, the harmonic indices can be expressed in terms of the *harmonic numbers* [19, 36]

$$\mathcal{H}_n = \sum_{k=1}^{n} \frac{1}{k} = 1 + \frac{1}{2} + \cdots + \frac{1}{n}.$$

Theorem 7.2. *The harmonic index of the antiregular graph A_{n+1} is*

$$\begin{aligned} h(A_{n+1}) = (2n+1)\mathcal{H}_{2n} + 2\mathcal{H}_{n+\lceil \frac{n}{2} \rceil} - \frac{5}{2}\mathcal{H}_n - (2n+1)\mathcal{H}_{2\lceil \frac{n}{2} \rceil} \\ + \frac{2n+1}{2}\mathcal{H}_{\lceil \frac{n}{2} \rceil} - n\mathcal{H}_{\lfloor \frac{n}{2} \rfloor} - n. \end{aligned} \tag{51}$$

Proof. For the first sum appearing in identity (50), we have

$$\sum_{k=0}^{\lfloor \frac{n-1}{2} \rfloor} \frac{1}{n+k+1} = \frac{1}{n+1} + \cdots + \frac{1}{n+\lfloor \frac{n-1}{2} \rfloor + 1} = \mathcal{H}_{n+\lfloor \frac{n-1}{2} \rfloor + 1} - \mathcal{H}_n.$$

For the second sum appearing in identity (50), we have

$$\begin{aligned} \sum_{k=0}^{n} \left\lfloor \frac{n-k}{2} \right\rfloor \frac{1}{n+k+1} &= \sum_{k=0}^{n} \left\lfloor \frac{k}{2} \right\rfloor \frac{1}{2n-k+1} \\ &= \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{k}{2n-2k+1} + \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \frac{k}{2n-2k} \\ &= \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n+\frac{1}{2}-\frac{1}{2}(2n-2k+1)}{2n-2k+1} + \frac{1}{2}\sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \frac{n-(n-k)}{n-k} \\ &= \left(n+\frac{1}{2}\right)\sum_{k=0}^{\lfloor n/2 \rfloor} \frac{1}{2n-2k+1} - \frac{1}{2}\left(\left\lfloor \frac{n}{2} \right\rfloor + 1\right) \\ &\quad + \frac{n}{2}\sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \frac{1}{n-k} - \frac{1}{2}\left(\left\lfloor \frac{n-1}{2} \right\rfloor + 1\right). \end{aligned}$$

For the two sums appearing in this last expression, we have

$$\begin{aligned} \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{1}{2n-2k+1} &= \frac{1}{2n+1} + \frac{1}{2n-1} + \cdots + \frac{1}{2n-2\lfloor n/2 \rfloor + 1} \\ &= \frac{1}{2n+1} + \frac{1}{2n-1} + \cdots + \frac{1}{2\lceil n/2 \rceil + 1} \\ &= \frac{1}{2n+1} + \frac{1}{2n} + \frac{1}{2n-1} + \cdots + \frac{1}{2\lceil n/2 \rceil + 2} + \frac{1}{2\lceil n/2 \rceil + 1} \\ &\quad - \frac{1}{2}\left(\frac{1}{n} + \cdots + \frac{1}{\lceil n/2 \rceil + 1}\right) \\ &= \mathcal{H}_{2n+1} - \mathcal{H}_{2\lceil n/2 \rceil} - \frac{1}{2}\left(\mathcal{H}_n - \mathcal{H}_{\lceil n/2 \rceil}\right) \end{aligned}$$

and

$$\sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \frac{1}{n-k} = \frac{1}{n} + \frac{1}{n-1} + \cdots + \frac{1}{n - \lfloor \frac{n-1}{2} \rfloor} = \mathcal{H}_n - \mathcal{H}_{n - \lfloor \frac{n-1}{2} \rfloor - 1} .$$

Furthermore, we have $\lfloor \frac{n}{2} \rfloor + \lfloor \frac{n-1}{2} \rfloor = n-1$ and $n - \lfloor \frac{n-1}{2} \rfloor - 1 = \lceil \frac{n}{2} \rceil$, for every $n \in \mathbb{N}$. Hence, we have

$$\begin{aligned} 2\sum_{k=0}^{n} \left\lfloor \frac{n-k}{2} \right\rfloor \frac{1}{n+k+1} &= (2n+1)\left(\mathcal{H}_{2n+1} - \mathcal{H}_{2\lceil n/2 \rceil} - \frac{1}{2}\left(\mathcal{H}_n - \mathcal{H}_{\lceil n/2 \rceil}\right)\right) \\ &\quad + n\left(\mathcal{H}_n - \mathcal{H}_{\lceil \frac{n}{2} \rceil}\right) - \left(\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{n-1}{2} \right\rfloor + 2 \right) \\ &= (2n+1)\mathcal{H}_{2n} + 1 - (2n+1)\mathcal{H}_{2\lceil n/2 \rceil} - \frac{1}{2}(2n+1)\mathcal{H}_n \\ &\quad + \frac{1}{2}(2n+1)\mathcal{H}_{\lceil n/2 \rceil} + n\mathcal{H}_n - n\mathcal{H}_{\lceil \frac{n}{2} \rceil} - (n-1+2) \\ &= (2n+1)\mathcal{H}_{2n} - (2n+1)\mathcal{H}_{2\lceil n/2 \rceil} - \frac{1}{2}\mathcal{H}_n + \frac{1}{2}(2n+1)\mathcal{H}_{\lceil n/2 \rceil} - n\mathcal{H}_{\lceil \frac{n}{2} \rceil} - n . \end{aligned}$$

In conclusion, we have the identity

$$\begin{aligned} h_{n+1} = 2\mathcal{H}_{n + \lfloor \frac{n-1}{2} \rfloor + 1} - 2\mathcal{H}_n + (2n+1)\mathcal{H}_{2n} - (2n+1)\mathcal{H}_{2\lceil n/2 \rceil} \\ - \frac{1}{2}\mathcal{H}_n + \frac{1}{2}(2n+1)\mathcal{H}_{\lceil n/2 \rceil} - n\mathcal{H}_{\lceil \frac{n}{2} \rceil} - n \end{aligned}$$

which simplifies in identity (51). □

The first values of the harmonic index h_n (for $n \geq 1$) are:

$$0,\ 1,\ \frac{4}{3},\ \frac{9}{5},\ \frac{226}{105},\ \frac{325}{126},\ \frac{13589}{4620},\ \frac{43177}{12870},\ \frac{335339}{90090},\ \frac{8431639}{2042040},\ \frac{261886013}{58198140},\ \frac{6484601}{1322685} .$$

8. Inverse sum index

In order to compute a first expression for the inverse sum index, we will use[2] another nice property of the antiregular graphs, i.e. the fact that they are split graphs. Recall that a *split graph* [14, 34] is a graph G whose vertex set V can be partitioned into two sets X and Y such that the induced subgraph on X is an independent set and the induced subgraph on Y is a complete graph. The partition $\{X,Y\}$ is a *split partition* of G. An antiregular graph A_n admit the *canonical split partition* $\{X_n,Y_n\}$, where the subset $X_n = \{1,2,\ldots,\lfloor n/2 \rfloor\}$ is independent

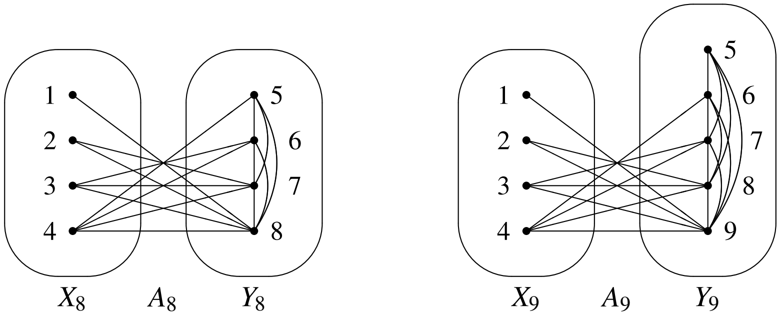

Figure 3: Canonical splitting of the antiregular graphs A_8 and A_9.

and the subset $Y_n = \{\lfloor n/2 \rfloor + 1, \lfloor n/2 \rfloor + 2, \dots, n\}$ induces a complete graph. See Figure 3 for two examples.

With respect to the canonical split partition of A_n, we have that the degree of an element of X_n is

$$d_n(k) = k \qquad \text{for } k = 1, 2, \dots, \lfloor n/2 \rfloor \tag{52}$$

and the degree of an element of Y_n is

$$d_n(\lfloor n/2 \rfloor + k) = \lfloor n/2 \rfloor - 1 + k \qquad \text{for } k = 1, 2, \dots, \lceil n/2 \rceil. \tag{53}$$

Then, we have the following result.

Theorem 8.1. *The inverse sum index of the antiregular graph A_n is*

$$\begin{aligned} I(A_n) = &\sum_{\substack{h,k=1 \\ h<k}}^{\lceil n/2 \rceil} \frac{(\lfloor n/2 \rfloor - 1 + h)(\lfloor n/2 \rfloor - 1 + k)}{2\lfloor n/2 \rfloor - 2 + h + k} \\ &+ \sum_{h=1}^{\lfloor n/2 \rfloor} \sum_{k=\lceil n/2 \rceil - h + 1}^{\lceil n/2 \rceil} \frac{h(\lfloor n/2 \rfloor - 1 + k)}{\lfloor n/2 \rfloor - 1 + h + k}. \end{aligned} \tag{54}$$

Proof. Consider the canonical split partition $\{X_n, Y_n\}$ of A_n. Then, by the definition of the inverse sum index, we immediately have the identity

$$\begin{aligned} I(A_n) = &\sum_{\substack{h,k=1 \\ h<k}}^{\lceil n/2 \rceil} \frac{d_n(\lfloor n/2 \rfloor + h)\, d_n(\lfloor n/2 \rfloor + k)}{d_n(\lfloor n/2 \rfloor + h) + d_n(\lfloor n/2 \rfloor + k)} \\ &+ \sum_{h=1}^{\lfloor n/2 \rfloor} \sum_{k=\lceil n/2 \rceil - h + 1}^{\lceil n/2 \rceil} \frac{d_n(h)\, d_n(\lfloor n/2 \rfloor + k)}{d_n(h) + d_n(\lfloor n/2 \rfloor + k)}. \end{aligned}$$

which simplifies in identity (54) by formulas (52) and (53). □

[2]This approach, clearly, can be used also in the other cases.

The first values of the inverse sum index I_n (for $n \geq 1$) are:

$$0, \frac{1}{2}, \frac{4}{3}, \frac{83}{20}, \frac{796}{105}, \frac{3653}{252}, \frac{309269}{13860}, \frac{75323}{2145}, \frac{804397}{16380}, \frac{56838385}{816816}, \frac{4262035621}{46558512}, \frac{1285453627}{10581480}.$$

In the next theorem, we give an alternative formula for the inverse sum index, by using a more formal approach.

Theorem 8.2. *The inverse sum index of the antiregular graph A_{n+2} is*

$$\begin{aligned} I_{n+2} = &\sum_{k=0}^{n} \left\lceil \frac{n-k}{2} \right\rceil \frac{n+k+2}{4} \\ &- \frac{1}{4} \sum_{k=0}^{n} \binom{n-k+2}{3} \frac{1}{n+k+2} + \left(\left\lfloor \frac{n}{2} \right\rfloor + 1 \right)^2 \\ &+ \left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - (n+2) \left\lfloor \frac{n}{2} \right\rfloor - 1 \right) \left(\mathcal{H}_{n+\lfloor n/2 \rfloor+2} - \mathcal{H}_{n+1} \right). \end{aligned} \tag{55}$$

Proof. By formula (12), the generating series of the inverse sum index of the antiregular graphs is

$$\sum_{n\geq 0} I(A_n)\, t^n = \int_0^1 \frac{\left[\Theta_x \Theta_y M(x,y;t)\right]_{x=y=q}}{q}\, \mathrm{d}q$$

where $M(x,y;t)$ is the generating series (42). Consider, for simplicity, the series

$$J(q;t) = \frac{\left[\Theta_x \Theta_y M(x,y;t)\right]_{x=y=q}}{q} \qquad \text{and} \qquad W(q;t) = \frac{q}{t^2} J(q;t/q).$$

By a straightforward calculation, we have

$$\begin{aligned} W(q;t) = &\frac{2t}{(1-t)^2(1+t)} \frac{1}{(1-qt)^3} + \frac{t^2+3t^3}{(1-t)^3(1+t)^2} \frac{1}{(1-qt)^2} \\ &+ \frac{2t^3+t^4+t^5}{(1-t)^4(1+t)^3} \frac{1}{1-qt} + \frac{4}{1-t} \frac{1}{(1-qt^2)^3} \\ &+ \frac{-3+t+5t^2}{(1-t)^3(1+t)} \frac{1}{(1-qt^2)^2} + \frac{t^3}{(1-t)^3(1+t)} \frac{1}{1-qt^2}. \end{aligned}$$

Since we have the expansions

$$\frac{t}{(1-t)^2(1+t)} = \sum_{n\geq 0} \left\lfloor \frac{n+1}{2} \right\rfloor t^n = \sum_{n\geq 0} \left\lceil \frac{n}{2} \right\rceil t^n \qquad [45, A004526]$$

$$\frac{t^2+3t^3}{(1-t)^3(1+t)^2} = \sum_{n\geq 0} \left\lceil \frac{n}{2} \right\rceil (n-1)\, t^n \qquad [45, A265225]$$

$$\frac{2t^3+t^4+t^5}{(1-t)^4(1+t)^3} = \sum_{n\geq 0}\left(\frac{n^2}{4}\left\lceil\frac{n}{2}\right\rceil - \frac{1}{4}\binom{n+2}{3}\right)t^n \qquad [45, A023856]$$

$$\frac{-3+t+5t^2}{(1-t)^3(1+t)} = \sum_{n\geq 0}\left(n-3+\left\lfloor\frac{n}{2}\right\rfloor\right)t^n \qquad [45, A032766]$$

$$\frac{t^3}{(1-t)^3(1+t)} = \sum_{n\geq 0}\left\lfloor\frac{n-1}{2}\right\rfloor\left\lceil\frac{n-1}{2}\right\rceil t^n \qquad [45, A002620],$$

then we have

$$\begin{aligned} W_n(q) = {} & 2\sum_{k=0}^{n}\left\lceil\frac{n-k}{2}\right\rceil\binom{k+2}{2}q^k + \sum_{k=0}^{n}\left\lceil\frac{n-k}{2}\right\rceil(n-k-1)\binom{k+1}{1}q^k \\ & + \sum_{k=0}^{n}\left(\frac{(n-k)^2}{4}\left\lceil\frac{n-k}{2}\right\rceil - \frac{1}{4}\binom{n-k+2}{3}\right)q^k \\ & + 4\sum_{k=0}^{\lfloor n/2\rfloor}\binom{k+2}{2}q^k + \sum_{k=0}^{\lfloor n/2\rfloor}\left(n-2k-3+\left\lceil\frac{n-2k}{2}\right\rceil\right)\binom{k+1}{1}q^k \\ & + \sum_{k=0}^{\lfloor n/2\rfloor}\left\lfloor\frac{n-2k-1}{2}\right\rfloor\left\lceil\frac{n-2k-1}{2}\right\rceil q^k. \end{aligned}$$

The general term of the first three sums is

$$\begin{aligned} & \left\lceil\frac{n-k}{2}\right\rceil(k+2)(k+1) + \left\lceil\frac{n-k}{2}\right\rceil(n-k-1)(k+1) \\ & \qquad + \frac{(n-k)^2}{4}\left\lceil\frac{n-k}{2}\right\rceil - \frac{1}{4}\binom{n-k+2}{3} = \\ & = \left\lceil\frac{n-k}{2}\right\rceil(k+1)(n+1) + \frac{(n-k)^2}{4}\left\lceil\frac{n-k}{2}\right\rceil - \frac{1}{4}\binom{n-k+2}{3} \\ & = \frac{(n+k+2)^2}{4}\left\lceil\frac{n-k}{2}\right\rceil - \frac{1}{4}\binom{n-k+2}{3} \end{aligned}$$

while the general term of the last three sums is

$$\begin{aligned} & 4\binom{k+2}{2} + \left(n-2k-3+\left\lceil\frac{n-2k}{2}\right\rceil\right)(k+1) + \left\lfloor\frac{n-2k-1}{2}\right\rfloor\left\lceil\frac{n-2k-1}{2}\right\rceil = \\ & = 2(k+2)(k+1) + \left(n-2k-3+\left\lceil\frac{n}{2}\right\rceil - k\right)(k+1) \\ & \qquad + \left(\left\lfloor\frac{n-1}{2}\right\rfloor - k\right)\left(\left\lceil\frac{n-1}{2}\right\rceil - k\right) \\ & = (k+1)\left(n-k+1+\left\lceil\frac{n}{2}\right\rceil\right) + \left(\left\lfloor\frac{n+1}{2}\right\rfloor - 1\right)\left\lfloor\frac{n}{2}\right\rfloor - (n-1)k + k^2 \end{aligned}$$

$$= n+k+1+k\left\lceil\frac{n}{2}\right\rceil + \left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil.$$

So, we have

$$\begin{aligned} W_n(q) = \sum_{k=0}^{n}\left(\frac{(n+k+2)^2}{4}\left\lceil\frac{n-k}{2}\right\rceil - \frac{1}{4}\binom{n-k+2}{3}\right)q^k \\ + \sum_{k=0}^{\lfloor n/2\rfloor}\left(n+k+1+\left\lfloor\frac{n}{2}\right\rfloor k + \left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil\right)q^k. \end{aligned}$$

Being $J(q;t) = qt^2 W(q;t)$, we have $J_{n+2}(q) = q^{n+1}W_n(q)$ and consequently

$$\begin{aligned} I_{n+2} &= \int_0^1 J_{n+2}(q)\,\mathrm{d}q = \int_0^1 q^{n+1}W_n(q)\,\mathrm{d}q \\ &= \sum_{k=0}^{n}\left\lceil\frac{n-k}{2}\right\rceil\left(\frac{(n+k+2)^2}{4} - \frac{1}{4}\binom{n-k+2}{3}\right)\frac{1}{n+k+2} \\ &\quad + \sum_{k=0}^{\lfloor n/2\rfloor}\left(n+k+1+\left\lfloor\frac{n}{2}\right\rfloor k + \left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil\right)\frac{1}{n+k+2} \\ &= \sum_{k=0}^{n}\left\lceil\frac{n-k}{2}\right\rceil\frac{n+k+2}{4} - \frac{1}{4}\sum_{k=0}^{n}\binom{n-k+2}{3}\frac{1}{n+k+2} \\ &\quad + \left(n+1+\left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil\right)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{1}{n+k+2} + \left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{k}{n+k+2}. \end{aligned}$$

Since

$$\sum_{k=0}^{\lfloor n/2\rfloor}\frac{k}{n+k+2} = \sum_{k=0}^{\lfloor n/2\rfloor}\frac{(n-k+2)-(n+2)}{n+k+2} = \left\lfloor\frac{n}{2}\right\rfloor + 1 - (n+2)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{1}{n+k+2}$$

and

$$\sum_{k=0}^{\lfloor n/2\rfloor}\frac{1}{n+k+2} = \frac{1}{n+2} + \cdots + \frac{1}{n+\lfloor n/2\rfloor+2} = \mathcal{H}_{n+\lfloor n/2\rfloor+2} - \mathcal{H}_{n+1},$$

we have

$$\left(n+1+\left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil\right)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{1}{n+k+2}+\left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{k}{n+k+2}=$$

$$=\left(n+1+\left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil\right)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{1}{n+k+2}$$

$$+\left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)\left(\left\lfloor\frac{n}{2}\right\rfloor+1-(n+2)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{1}{n+k+2}\right)$$

$$=\left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)^2+\left(\left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil-(n+2)\left\lfloor\frac{n}{2}\right\rfloor-1\right)\sum_{k=0}^{\lfloor n/2\rfloor}\frac{1}{n+k+2}$$

$$=\left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)^2+\left(\left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil-(n+2)\left\lfloor\frac{n}{2}\right\rfloor-1\right)\left(\mathcal{H}_{n+\lfloor n/2\rfloor+2}-\mathcal{H}_{n+1}\right).$$

In conclusion, we have formula (55). □

Formula (55) can be further simplified. To do that, we need the following two lemmas.

Lemma 8.3. *We have the identity*

$$\sum_{k=0}^{n}\left\lceil\frac{n-k}{2}\right\rceil(n+k+2)=(n+2)\left\lceil\frac{n}{2}\right\rceil\left\lceil\frac{n+1}{2}\right\rceil+\frac{n(n+1)(2n+1)}{24}-\frac{1}{4}\left\lceil\frac{n}{2}\right\rceil. \tag{56}$$

Proof. By replacing k with $n-k$, we have

$$\sum_{k=0}^{n}\left\lceil\frac{n-k}{2}\right\rceil(n+k+2)=\sum_{k=0}^{n}\left\lceil\frac{k}{2}\right\rceil(n+2+n-k)$$

$$=(n+2)\sum_{k=0}^{n}\left\lceil\frac{k}{2}\right\rceil+\sum_{k=0}^{n}\left\lceil\frac{k}{2}\right\rceil(n-k).$$

For the first sum, we have the generating series

$$\sum_{n\geq 0}\left(\sum_{k=0}^{n}\left\lceil\frac{k}{2}\right\rceil\right)t^n=\frac{1}{1-t}\sum_{n\geq 0}\left\lceil\frac{n}{2}\right\rceil t^n$$

$$=\frac{t}{(1-t)^3(1+t)}=\sum_{n\geq 0}\left\lfloor\frac{n+1}{2}\right\rfloor\left\lceil\frac{n+1}{2}\right\rceil t^n$$

and so

$$\sum_{k=0}^{n}\left\lceil\frac{k}{2}\right\rceil=\left\lceil\frac{n}{2}\right\rceil\left\lceil\frac{n+1}{2}\right\rceil.$$

Similarly, for the second sum, we have the generating series

$$\begin{aligned}\sum_{n\geq 0}\left(\sum_{k=0}^{n}\left\lceil\frac{k}{2}\right\rceil(n-k)\right)t^n &= \sum_{n\geq 0} n\,t^n\cdot\sum_{n\geq 0}\left\lceil\frac{n}{2}\right\rceil t^n\\ &= \frac{t}{(1-t)^2}\cdot\frac{t}{(1-t)^2(1+t)} = \frac{t^2}{(1-t)^4(1+t)}\,.\end{aligned}$$

This is the generating series of sequence A002623, and so

$$\sum_{k=0}^{n}\left\lceil\frac{k}{2}\right\rceil(n-k) = \frac{n(n+1)(2n+1)}{24} - \frac{1}{4}\left\lceil\frac{n}{2}\right\rceil.$$

Hence, we have identity (56). □

Lemma 8.4. *We have the identity*

$$\begin{aligned}\sum_{k=0}^{n}\binom{n-k+2}{3}\frac{1}{n+k+2} &= \frac{2}{3}(n+1)(n+2)(2n+3)(\mathcal{H}_{2n+1}-\mathcal{H}_n)\\ &\quad -\frac{1}{9}(n+2)(8n^2+23n+18)\,.\end{aligned} \tag{57}$$

Proof. First, we rewrite our sum as follows

$$\sum_{k=0}^{n}\binom{n-k+2}{3}\frac{1}{n+k+2} = \sum_{k=0}^{n}\binom{k+2}{3}\frac{1}{2n-k+2} = \frac{1}{6}\sum_{k=0}^{n}\frac{k^3+3k^2+2k}{2n-k+2}\,.$$

Now, we express the polynomial k^3+3k^2+2k as a linear combination of powers of $2n-k+2$. Let $\alpha = 2n+2$. Then, we have

$$\begin{aligned}k^3+3k^2+2k &= (\alpha-(\alpha-k))^3+3(\alpha-(\alpha-k))^2+2(\alpha-(\alpha-k))\\ &= -(\alpha-k)^3+3(\alpha+1)(\alpha-k)^2-(3\alpha^2+6\alpha+2)(\alpha-k)+(\alpha+2)(\alpha+1)\alpha\\ &= -(2n-k+2)^3+3(2n+3)(2n-k+2)^2-2(6n^2+18n+13)(2n-k+2)\\ &\qquad +4(n+1)(n+2)(2n+3)\,.\end{aligned}$$

Moreover, we have

$$\begin{aligned}\sum_{k=0}^{n}\frac{1}{2n-k+2} &= \frac{1}{2n+2}+\cdots+\frac{1}{n+2}\\ &= \mathcal{H}_{2n+2}-\mathcal{H}_{n+1} = \mathcal{H}_{2n+1}-\mathcal{H}_n-\frac{1}{2}\,\frac{1}{n+1}\,.\end{aligned}$$

Using these identities, we have

$$
\begin{aligned}
\sum_{k=0}^{n} \frac{k^3+3k^2+2k}{2n-k+2} &= \\
&= \sum_{k=0}^{n} \big(-(2n-k+2)^2 + 3(2n+3)(2n-k+2) - 2(6n^2+18n+13) \big) \\
&\qquad + 4(n+1)(n+2)(2n+3) \sum_{k=0}^{n} \frac{1}{2n-k+2} \\
&= 4(n+1)(n+2)(2n+3) \left(\mathcal{H}_{2n+1} - \mathcal{H}_n - \frac{1}{2}\,\frac{1}{n+1} \right) \\
&\qquad - \sum_{k=0}^{n} \big(k^2 + (2n+5)k + 2(2n^2+7n+6) \big) \\
&= 4(n+1)(n+2)(2n+3)(\mathcal{H}_{2n+1} - \mathcal{H}_n) - 2(n+2)(2n+3) \\
&\qquad - \left(\frac{n(n+1)(2n+1)}{6} + (2n+5)\binom{n+1}{2} + 2(2n^2+7n+6)(n+1) \right) \\
&= 4(n+1)(n+2)(2n+3)(\mathcal{H}_{2n+1} - \mathcal{H}_n) - \frac{2}{3}\,(8n^3+39n^2+64n+36).
\end{aligned}
$$

So, we have identity (57). □

Finally, by identities (55), (56) and (57), we have (after some simplifications) the following closed form for the inverse sum index of the connected antiregular graphs.

Theorem 8.5. *The inverse sum index of the antiregular graph A_{n+2} is*

$$
\begin{aligned}
I_{n+2} = &\left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - (n+2) \left\lfloor \frac{n}{2} \right\rfloor - 1 \right) (\mathcal{H}_{n+\lfloor n/2 \rfloor+2} - \mathcal{H}_{n+1}) \\
&- \frac{1}{6}\,(n+1)(n+2)(2n+3)(\mathcal{H}_{2n+1} - \mathcal{H}_n) \\
&+ \frac{n+2}{4} \left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{n}{2} \right\rfloor^2 - \frac{4n-25}{16} \left\lfloor \frac{n}{2} \right\rfloor \\
&+ \frac{70n^3+393n^2+641n+576}{288}.
\end{aligned}
\tag{58}
$$

We conclude with the following asymptotic expansion.

Theorem 8.6. *For $n \to +\infty$, we have the asymptotic expansion*

$$
I(A_n) \sim \left(\frac{11}{36} - \frac{\ln 2}{3} \right) n^3 \simeq 0.0745065\, n^3\,. \tag{59}
$$

Proof. We will use the following property: let $\alpha = \{a_n\}_{n\in\mathbb{N}}$ and $\beta = \{b_n\}_{n\in\mathbb{N}}$ be two real sequences such that $a_n,\, b_n > 0$ and $a_n \le b_n$ for all $n \in \mathbb{N}$, and

$$\lim_{n\to+\infty} a_n = +\infty \qquad \text{and} \qquad \lim_{n\to+\infty} \frac{b_n}{a_n} = L \in \mathbb{R}\,.$$

Then, for the numbers

$$\mathcal{H}_n^{(\alpha,\beta)} = \sum_{k=a_n}^{b_n} \frac{1}{k} = \mathcal{H}_{b_n} - \mathcal{H}_{a_n-1}\,,$$

we have

$$\lim_{n\to+\infty} \mathcal{H}_n^{(\alpha,\beta)} = \ln L\,.$$

By this property, we have the limits

$$\lim_{n\to+\infty} (\mathcal{H}_{n+\lfloor n/2\rfloor+2} - \mathcal{H}_{n+1}) = \ln\frac{3}{2} \qquad \text{and} \qquad \lim_{n\to+\infty} (\mathcal{H}_{2n+1} - \mathcal{H}_n) = \ln 2\,.$$

Hence, by formula (58), we obtain straightforwardly the asymptotic expansion (59). □

Remark 8.7. Notice that, with a similar argument, we can obtain the asymptotic expansion also for the harmonic index. Indeed, being

$$\begin{aligned} h(A_{n+1}) = {} & 2\Big(\mathcal{H}_{n+\lfloor\frac{n-1}{2}\rfloor+1} - \mathcal{H}_n\Big) \\ & + (2n+1)\left(\mathcal{H}_{2n+1} - \mathcal{H}_{2\lceil\frac{n}{2}\rceil} - \frac{1}{2}(\mathcal{H}_n - \mathcal{H}_{\lceil\frac{n}{2}\rceil})\right) \\ & + n\Big(\mathcal{H}_n - \mathcal{H}_{n-\lfloor\frac{n-1}{2}\rfloor-1}\Big) - n - 1\,, \end{aligned}$$

we have

$$h(A_n) \sim (2\ln 2 - 1)\,n \qquad \text{as } n \to +\infty\,.$$

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E. MUNARINI
Dipartimento di Matematica
Politecnico di Milano
e-mail: `emanuele.munarini@polimi.it`