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On Zagreb Indices of Pseudo-regular Graphs

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ABSTRACT. Properties of the Zagreb indices of pseudo-regular graphs are established, with emphasis on the Zagreb indices inequality. The relevance of the results obtained for the theory of nanomolecules is pointed out.

1. INTRODUCTION: ZAGREB INDICES

Let G be a graph with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)=\{e_1,e_2,\ldots,e_m\}$, thus possessing n vertices and m edges. The degree $d(v)$ of the vertex $v\in V(G)$ is the number of first neighbors of v. The edge of the graph G, connecting the vertices u and v, will be denoted by uv. Throughout this paper, the graphs considered are assumed to be connected.

In mathematical chemistry, two simple graph invariants

$$M_1 = M_1(G) := \sum_{v\in V(G)} d(v)^2 \qquad \text{and} \qquad M_2 = M_2(G) := \sum_{uv\in E(G)} d(u)d(v)$$

were first time encountered in connection with the study of the structure-dependency of total π-electron energy [1] and soon thereafter used for modeling of branching-based properties of alkanes [2]. Eventually, these two structure-descriptors where

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named *Zagreb group indices* [3]. Nowadays these are commonly referred to as the *first* (M_1) and *second* (M_2) *Zagreb indices.*

For information on the two Zagreb indices and a number of similar molecular structure descriptors, the readers should consult the books [4-6] and/or the reviews [7-11]. Of the countless published papers on Zagreb indices, we mention only the most recent ones [12-32], in which references to earlier works can be found.

2. INTRODUCTION: PSEUDO-REGULAR GRAPHS

Let $m(u)$ be the average degree of the vertices adjacent to the vertex $u \in V(G)$, that is,

$$m(u) := \frac{1}{d(u)} \sum_{uv \in E(G)} d(v).$$

Define by

$$\langle m(G) \rangle = \frac{1}{n} \sum_{u \in V(G)} m(u)$$

the average neighbor degree number of the graph G.

A graph is said to be regular (of degree r) is all its vertices are of equal degree (equal to r). A graph is called pseudo-regular [33,34] if there exists a positive constant $p = p(G)$, such that the average degree of each vertex of G is equal to p. Of course, every regular graph is also pseudo-regular. There, however, exist pseudo-regular graphs in which the vertex degrees assume N different values for $N = 2$ (biregular graphs), N = 3(triregular graphs), N = 4, etc. Two examples are given in Fig. 1.

The relevance of pseudo-regular graphs for the theory of nanomolecules and nanostructures should become evident from the following. There exist polyhedral (planar, 3-connected) graphs and infinite periodic planar graphs belonging to the family of the pseudo-regular graphs.

Among polyhedra, the deltoidal hexecontahedron possesses this property, see Fig.2. Its edge-graph is pseudo-regular with p = 4. The deltoidal hexecontahedron is a Catalan polyhedron with 60 deltoid faces, 120 edges, and 62 vertices, with degrees 3, 4, and 5. Its 62 vertices are characterized by the following vertex degree distribution: $n_3 = 20$, $n_4 = 30$, and $n_5 = 12$. The average degree of its vertices is 240/62 =3.87968 .

An exceptional property of the deltoidal hexecontahedron is that in each vertex, the average degrees of the neighbor vertices is equal to 4. Indeed, the average neighbor degree number of the edge graph G_H of the deltoidal hexecontahedron is

$$\langle m(G_H)\rangle = \frac{1}{n}\sum_{u\in V(G)} m(u) = \frac{1}{62}\left(20\cdot\frac{4+4+4}{3} + 30\cdot\frac{3+5+3+5}{4} + 12\cdot\frac{4+4+4+4+4}{5}\right)$$

$$= \frac{1}{62}\left(20\cdot 4 + 30\cdot 4 + 12\cdot 4\right) = \frac{62\cdot 4}{62} = 4.$$

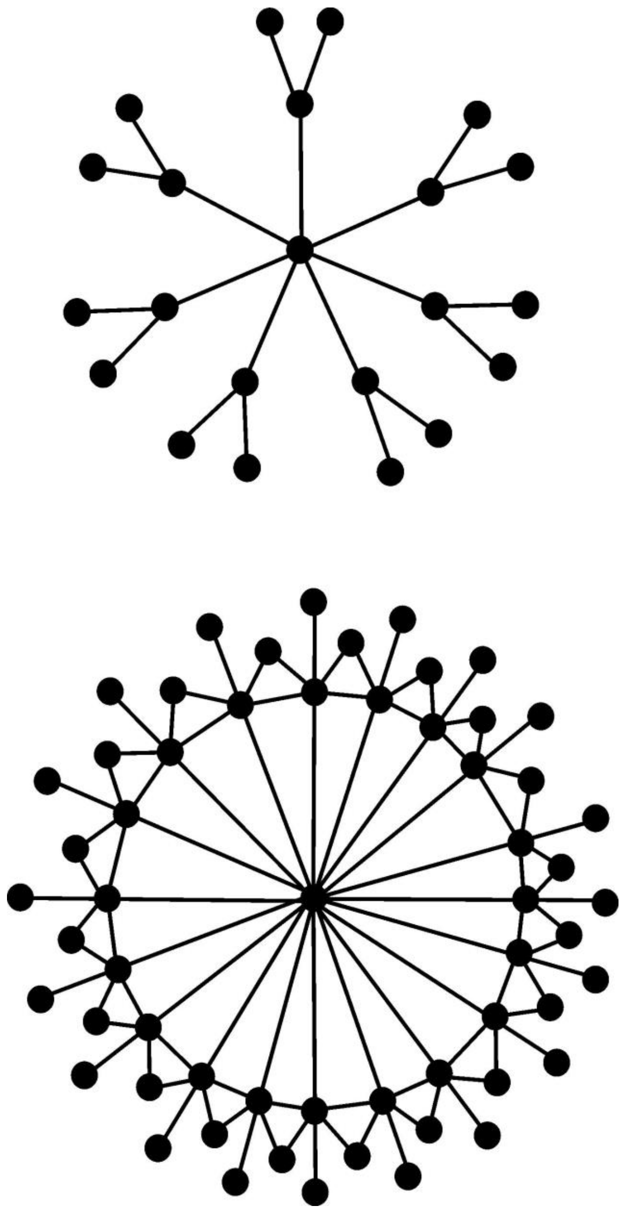

Fig. 1. Examples of pseudo-regular graphs. For the top graph N = 3, the central vertex must have degree equal to $p^2 - p + 1$, and here p = 3. For the bottom graph N = 4, the central vertex must have degree equal to $p^2 - 3p + 1$, and here p= 6.

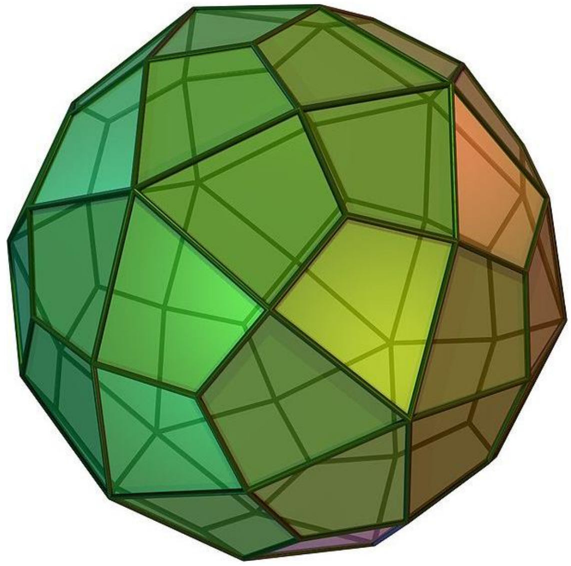

Fig. 2. The deltoidal hexecontahedron; for details see text.

A variety of other chemically relevant polyhedra and polyhedra-type structures, whose graphs are pseudo-regular, can be found in the books [35-37] and other works by Diudea. Therefore, the study of the properties of pseudo-regular graphs may be of some value for nano-science.

3. RELATIONS BETWEEN THE ZAGREB INDICES OF PSEUDO-REGULAR GRAPHS

We first recall that in the case of regular graphs (and thus for the molecular graphs of fullerenes and the majority of nanotubes and similar nanomolecules), the structure-dependency of the two Zagreb indices is trivial:

$$M_1 = nr^2 = 2mr \qquad \text{and} \qquad M_2 = mr^2 = \frac{1}{2}nr^3$$

where, as before, n and m are, respectively, the number of vertices and edges, whereas r is the degree of any vertex. In chemically relevant cases, r=3.

In the case of pseudo-regular graphs, the situation with the Zagreb indices is somewhat less simple.

We start with two previously established lemmas.

Lemma 1. [30] Denote by $[d(G)]$ the average degree of G. For a connected simple graph G, the inequality $\langle m(G)\rangle \geq 2m/n = [d(G)]$ holds, with equality if and only if G is regular.

Lemma 2. [38] For a connected graph G

$$M_1(G) = \sum_{u \in V(G)} m(u)d(u)$$

and

$$2M_2(G) = \sum_{u \in V(G)} m(u)d(u)^2 .$$

Proposition 1. If G is pseudo-regular, i. e., $m(u) = p$ holds for all $u \in V(G)$, then

$$p(G) = \langle m(G) \rangle = \frac{2M_2(G)}{M_1(G)} \geq [d(G)] \tag{1}$$

with equality if and only if G is regular.

Proof. The inequality (1) is the consequence of Lemma 2. From this it follows that for a pseudo-regular graph G, the relations $M_1(G) = 2mp$ and $M_2(G) = mp^2$ hold. ■

Consider now the graph invariant $T(G)$, defined as

$$T = T(G) := \frac{mM_1(G)}{nM_2(G)} . \tag{2}$$

It follows that $T \leq 1$ if and only if, $M_1/n \leq M_2/m$, and T<1 if and only if, $M_1/n < M_2/m$.

Recall that the inequality $M_1/n \leq M_2/m$ was subject of numerous studies, starting with [39]. It is often referred to as the *Zagreb indices inequality.* For details see the reviews [10,11], the recent papers [13-17,21,23,24,27-29,31,32], and the references cited therein.

Proposition 2. If the graph G is pseudo-regular, but not regular, then the *strict Zagreb indices inequality* ($M_1/n \leq M_2/m$) holds.

Proof. From Eqs. (1) and (2) it follows that

$$T(G) = \frac{mM_1(G)}{nM_2(G)} = [d(G)]\frac{M_1(G)}{2M_2(G)} = \frac{[d(G)]}{p(G)} \leq 1 \tag{3}$$

and equality is attained in (3) if and only if G is regular. Consequently, the inequality (3) is strict if G is a non-regular pseudo-regular graph. ■

We now pay attention to a special class of pseudo-regular graphs, denoted by $G(p)$, whose one representative is depicted in Fig. 3. For these graphs, p = 4, 5, 6, …, and the central vertex has degree $p^2 - 3p + 3$. It is easy to verify that the average vertex degree of $G(p)$ is:

$$\left[d(G(p))\right] = \frac{2m}{n} = \frac{2(p-1)(p^2-3p+3)}{1+(p-2)(p^2-3p+3)}$$

from which it immediately follows $\lim_{p\to\infty}\left[d(G(p))\right] = 2$, implying

$$\lim_{p\to\infty} T(G(p)) = \lim_{p\to\infty} \frac{\left[d(G(p))\right]}{p} = 0\,. \tag{4}$$

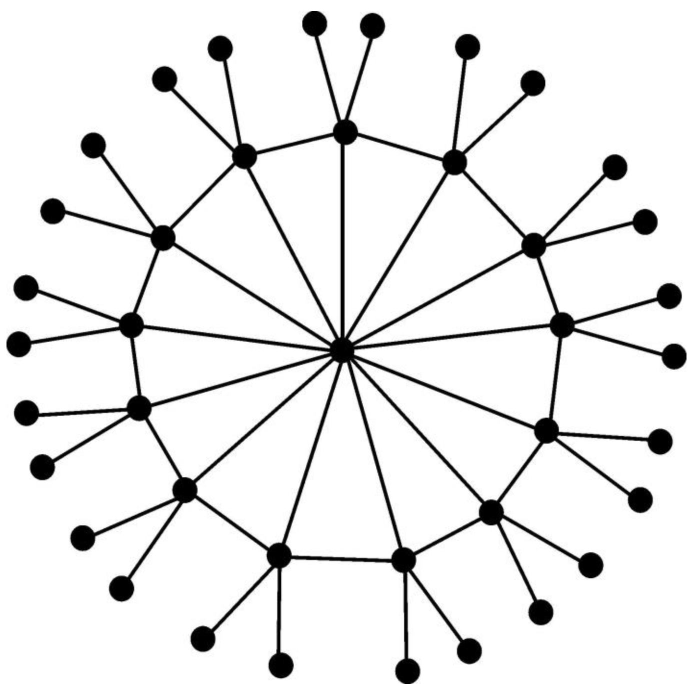

Fig. 3. A connected triregular pseudo-regular graph, denoted by $G(p)$; here: p = 5.

From relation (4) we deduce the following:

Proposition 3. It is possible to construct connected graphs for which the invariant $T(G)$ is an arbitrary small positive number and tends to zero as $n \to \infty$. The sequence $G(5), G(6), G(7), \ldots$ provides an example of such graphs. More specifically, for the graphs $G(p)$, shown is Fig. 3,

$$\frac{M_1(G(p))}{n}=\frac{2(p^2-3p+3)(p-1)p}{(p^2-3p+3)(p-2)+1} \quad \text{and} \quad \frac{M_2(G(p))}{m}=p^2$$

and therefore both M_1/n and M_2/m tend to infinity as p (or n or m) tend to infinity. However, for $p \to \infty$, the quotient of $M_1(G(p))/n$ and $M_2(G(p))/m$ tends to zero.

Proposition 4. If G is pseudo-regular, i. e., $m(u) = p$ holds for all $u \in V(G)$, and if m is the number of its edges, then

$$M_1(G)=\frac{M_2(G)}{p}+mp\,. \tag{5}$$

Proof. For a pseudo-regular graph G, the following relations hold: $M_1(G) = 2mp$ and $M_2(G) = mp^2$. From this, the claim follows. ■

In connection with Eq. (5) we make the following observation. There exists a particular class Π of connected graphs, characterized by the following property: For any $G \in \Pi$ with edge number m, there exists a positive number $p = p(G)$, such that

$$M_1(G)=\frac{M_2(G)}{P}+mP \tag{6}$$

holds. It may be that $p(G)$ is always a positive integer.

According to our considerations, the following graphs are included in the class Π:

a) P-dominant graphs (having one or two dominant degrees); see [31] for details
b) Pseudo-regular graphs
c) In addition, there exist connected graphs that are neither P-dominant nor pseudo-regular, belonging to the class Π.

To demonstrate the case c), consider the triregular graph G_D, depicted in Fig. 4, having degree set $D(G_D)=\{3,4,5\}$. For this graph, $n(G_D)=7$, $m(G_D) = 12$, $M_1(G_D) = 86$, and $M_2(G_D) = 152$. It is easy to check that G_D has no domination degree [31], and is not pseudo-regular. Nevertheless, for $p = 4$, the equality (6) is obeyed:

$$M_1(G_D)=\frac{M_2(G_D)}{4}+4m(G_D)=\frac{152}{4}+4\cdot 12=86.$$

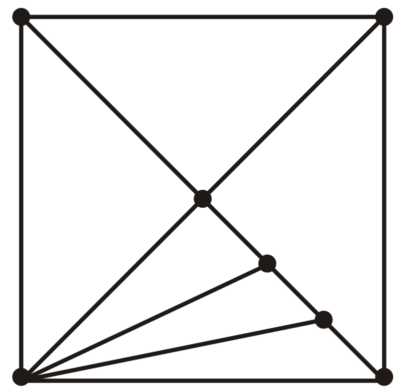

Fig. 4. A non-pseudo-regular and non P-dominant graph G_D, satisfying identity (6).
In connection with relation (6) we have some further observations.

Proposition 5. A connected or disconnected graph G belongs to class Π if and only if inequality $M_1^2(G) - 4mM_2 \geq 0$ holds.

Proof. Starting with equation (6), consider the polynomial function of second degree $Z_G(p)$ defined as

$$Z_G(P) = mP^2 - M_1P + M_2$$

It is easy to see that if $Z_G(p)$ has real roots (one or two), then these are positive numbers. Moreover, the function $Z_G(p)$ has (one or two) positive roots if and only if, $M_1^2(G) - 4mM_2 \geq 0$ holds for its discriminant. ■

Lemma 3. [40] Let G be a simple connected graph. Then,

$$M_2 \geq \frac{4m^3}{n^2} .$$

The equality is attained if and only if graph is regular.

Proposition 6. Let G be a connected graph satisfying the Zagreb indices equality, i. e., let the condition $M_1(G)/n = M_2(G)/m$ hold. Then there exists a positive number P that satisfies identity (6).

Proof. If there is a number P that satisfies Eq.(6) , then

$$\frac{n}{m}M_2 = \frac{M_2}{P} + mP$$

should be fulfilled. This leads to the polynomial function $J_G(P)$ of second degree, given as

$$J_G(P) = mP^2 - \frac{nM_2}{m}P + M_2$$

It is enough to verify that for the discriminant of $J_G(P)$ the inequality

$$\left(\frac{nM_2}{m}\right)^2 - 4mM_2 = M_2\left(\frac{n^2}{m^2}M_2 - 4m)\right) \geq 0$$

holds. From Lemma 3, it follows that

$$\left(\frac{n^2}{m^2}M_2 - 4m)\right) \geq 0$$

with equality if and only if G is regular. This implies the claim. ∎

We say that a graph G is k-end-degree regular if there exists a positive integer k, such that condition $d(u)+d(v)=k$ holds for each edge $uv \in E(G)$.

Proposition 7. For each k-end-degree regular graph, there is a positive number P, such that Eq. (6) is obeyed.

Proof. If there is a number P that satisfies Eq. (6), then it is obviously positive since the left-hand side of Eq. (6) is positive and its right hand-side is of the same sign as P. Hence, it is enough to show that $M_1{}^2 - 4mM_2 \geq 0$. It holds:

$$M_1{}^2 - 4mM_2 = \left(\sum_{u\in V(G)} d(u)^2\right)^2 - 4m\sum_{uv\in E(G)} d(u)d(v)$$

$$= \left(\sum_{u\in V(G)}\sum_{v:uv\in E(G)} d(u)\right)^2 - 4m\sum_{uv\in E(G)} d(u)d(v)$$

$$= \left(\sum_{uv\in E(G)} \left(d(u)+d(v)\right)\right)^2 - 4m\sum_{uv\in E(G)} d(u)d(v)$$

$$= m^2k^2 - 4m\sum_{uv\in E(G)} d(u)[k-d(u)] = m\sum_{uv\in E(G)}\left(k^2 - 4d(u)[k-d(u)]\right).$$

Consider the function $f(x) = x \cdot (k - x)$. Simple analysis shows that its maximum is at $x = k/2$ and that $f(x) \le k^2/4$. Therefore

$$m \sum_{uv \in E(G)} \left(k^2 - 4d(u)[k - d(u)]\right) \ge m \sum_{uv \in E(G)} \left(k^2 - 4 \cdot \frac{k^2}{4}\right) = 0 .$$

This proves the Proposition. ■

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