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# On the Relations between the Zagreb Indices, Clique Numbers and Walks in Graphs

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#### Abstract

Abdo et al. demonstrated [MATCH Commun. Math. Comput. Chem. **72** (2014) 741-751] that there exist connected graphs for which  $\mu^2(G) \approx M_2(G)/m$  where  $\mu(G)$  is the spectral radius of a graph G,  $M_2(G)$  is the second Zagreb index and m the number of edges. We use and extend this approximation to investigate opportunities to convert results from spectral graph theory into results involving the first and the second Zagreb indices  $M_1(G)$  and  $M_2(G)$ . We do this principally by noting that  $M_1(G)=w_3$  and  $2M_2(G)=w_4$ , where  $w_3$  and  $w_4$  are the numbers of 3- and 4-walks in a graph, respectively.

### 1. Introduction

Let G=G(V,E) be a graph with vertex set V(G) and edge set E(G). Denote by n and m the number of vertices and edges of G, respectively. To avoid trivialities we always assume that  $n\geq 2$ . An edge of G connecting vertices u and v is denoted by uv. For a vertex u, d(u) denotes the degree of u and d=d(G)=2m/n the average degree of G. We denote by  $\Delta=\Delta(G)$  and  $\delta=\delta(G)$  the maximum and the minimum degrees, respectively, of vertices of G. A graph is called regular (R-regular), if all its vertices have the same degree R. A connected graph with maximum vertex degree at most 4 is said to be a chemical graph.

Using the standard terminology [1], let A=A(G) denote the adjacency matrix of G,  $\mu=\mu(G)$  the spectral radius of G, and  $\omega(G)$  the clique number of G. The average-degree of the vertices adjacent to a vertex u is defined as  $d_{av}(u)=D_2(u)/d(u)$ , where  $D_2(u)$  is the sum of degrees of the vertices adjacent to u. A graph G is called harmonic (pseudoregular) if the average-degree  $d_{av}(u)$  is equal for any vertex u. If G is harmonic then the average-degree is identical to the spectral radius of G. Moreover, a graph G is harmonic if and only if  $A^2j = \mu Aj$  holds, where j is the all-one vector [2,3].

Define the first and second Zagreb indices of a graph G as usual as follows [4-12]:

$$\mathbf{M}_1 = \mathbf{M}_1(\mathbf{G}) = \sum_{u \in V} \mathbf{d}^2(u) \quad \text{and} \qquad \mathbf{M}_2 = \mathbf{M}_2(\mathbf{G}) = \sum_{u v \in E} \mathbf{d}(u) \mathbf{d}(v)$$

For more detailed information on Zagreb indices, we refer the reader to surveys [13-16]. For a graph G, a k-walk is a sequence of vertices  $v_1, \ldots, v_k$  such that  $v_i$  is adjacent to  $v_{i+1}$  for all i=1,2,...k-1. We denote by  $w_k = w_k(G)$  the number of k-walks in G [2,3]. Teranishi [17] has noted that:

$$w_1=n$$
,  $w_2=2m$ ,  $w_3=M_1(G)$  and  $w_4=2M_2(G)$ .

Denote by  $\alpha(G)$  and  $\beta(G)$  two distinct topological invariants of a graph G. Throughout this paper  $\alpha(G) \approx \beta(G)$  will mean that there exists a family  $\Omega$  of graphs which includes graphs  $G_1$ ,  $G_2$  and  $G_3$  for which  $\alpha(G_1)=\beta(G_1)$ ,  $\alpha(G_2) < \beta(G_2)$  and  $\alpha(G_3) > \beta(G_3)$  hold. Abdo et al. [16] demonstrated experimentally that for the set of connected have graphs  $\mu^2(G) \approx M_2(G) / m = w_4(G) / w_2(G)$  . They provide examples of graphs for which  $\mu^2 = M_2 / m_{\star}$  $\mu^2$ < M<sub>2</sub>/m, and  $\mu^2$  > M<sub>2</sub>/m hold.

In this paper, we investigate and characterize some classes of graphs for which the relation  $\mu^r(G) \approx w_{r+q} / w_q$  is fulfilled. It is verified that this relation is valid for graphs with no isolated vertices when q is even, moreover, if G is harmonic, the equality  $\mu^r(G)=w_{r+q}(G)/w_q(G)$  holds for arbitrary r≥1 and q≥2. Using the Motzkin-Straus theorem a general lower bound for the clique number  $\omega(G)$  is established. We derive a novel upper bound for the second variable Zagreb index  ${}^{s}M_2(G)$  and answer a question due to Nikiforov. We begin, however, with a series of new lower bounds for  $\omega(G)$ , one of which uses the second Zagreb index  $M_2(G)$ .

## **2.** Lower bounds for ω(G)

Zhou [10] proved the following upper bounds for  $M_1$  and  $M_2$  as a function of  $\omega(G)$ .

#### Theorem 1.

$$M_1(G) \le \frac{\omega - 1}{\omega} 2nm \tag{1}$$

$$M_{2}(G) \le \frac{2}{\omega}m^{2} + \frac{(\omega-1)(\omega-2)}{\omega^{2}}n^{2}m$$
(2)

These bounds are sharp if and only if G is a complete bipartite or a regular complete q-partite graph. An alternative proof of (1) is available from Theorem (2) since Edwards and Elphick [18] noted that that  $\mu^2 \ge M_1/n$ .

The following sequence of lower bounds for the clique number is reasonably well known. **Theorem 2.** 

$$\frac{n}{n-d} \le \frac{n}{n-\mu} \le \frac{2m}{2m-\mu^2} \le \omega(G)$$

The weakest bound is due to Myers and Liu [19], the middle bound to Wilf [20], and the strongest bound to Nikiforov [21]. The following Theorem provides a degree-based alternative to the Nikiforov bound.

Theorem 3. Let G be any graph. Then for arbitrary values of S

$$g(S) = \frac{\left(\sum_{u \in V} d^{S}(u)\right)^{2}}{\left(\sum_{u \in V} d^{S}(u)\right)^{2} - 2\sum_{u v \in E} d^{S}(u)d^{S}(v)} \le \omega(G)$$
(3)

Proof. The Motzkin-Straus [22] inequality can be interpreted as follows. If G is a graph with a clique number  $\omega(G)$ , then for any n-vector  $(x_1, x_2, \dots x_n)$  with  $x_i \ge 0$  for all i, and  $x_1 + x_2 + \dots + x_n = 1$ :

$$\sum_{[i,j]\in E} x_i x_j \le \frac{\omega - 1}{2\omega}$$

Let  $V(G) = \{u_1, u_2, \dots, u_n\}$  be the vertex set of G, and define  $x_i$  as follows:

$$\mathbf{x}_{i} = \mathbf{d}^{s}(\mathbf{u}_{i}) / \sum_{\mathbf{u} \in \mathbf{V}} \mathbf{d}^{s}(\mathbf{u})$$

Therefore  $x_1 + x_2 +, \dots, + x_n = 1$ , this implies that

$$\sum_{uv\in E} d^{s}(u)d^{s}(v) = \left(\sum_{u\in V} d^{s}(u)\right)^{2} \sum_{\{i,j\}\in E} x_{i}x_{j} \le \left(\sum_{u\in V} d^{s}(u)\right)^{2} \frac{(\omega-1)}{2\omega}.$$
(4)

Corollary 1. With S=0 we reproduce the Myers and Liu bound, namely

$$\frac{n^2}{n^2 - 2m} \le \omega(G) \cdot$$

Corollary 2. With S=1 we obtain

$$M_2 = \sum_{u \in E} d(u)d(v) = 4m^2 \sum_{\{i,j\} \in E} x_i x_j \le 2m^2 \frac{(\omega - 1)}{\omega} \quad \text{ or equivalently } \quad \frac{2m^2}{2m^2 - M_2} \le \omega(G) + \frac$$

The bound is sharp for complete bipartite graphs and for regular complete q-partite graphs. Note that it is immediate that for triangle-free graphs  $M_2 \le m^2$  as proved by Zhou [10]. Moreover, combining this corollary with (1) we observe that

$$\max\left\{\frac{M_1}{n}, \frac{M_2}{m}\right\} \le 2m\frac{(\omega-1)}{\omega}$$

Corollary 3. With S=2 one obtains

$$\sum_{uv\in E} d^2(u)d^2(v) \le M_1^2 \frac{(\omega-1)}{2\omega}.$$

**Corollary 4.** Let G be a chemical graph, other than  $K_{5}$ . Then  $M_2(G) \le 1.5m^2$ . Proof. For a chemical graph  $\Delta \le 4$  holds. It follows from Brooks' [23] famous theorem that, excluding  $K_5$ ,  $\omega(G) \le \Delta \le 4$ . Therefore

$$M_2 \le \frac{(\omega - 1)}{\omega} 2m^2 \le \frac{3}{4} 2m^2 = 1.5m^2$$

This bound is sharp, for example, for K<sub>4</sub> complete graph.

**Corollary 5.** It is easy to see that  $g(0) \le g(1)$ . Moreover, there exist graphs with g(S) > g(1) for some S > 1. For these graphs the series of lower bounds for  $\omega(G)$  initially increases as S increases. This phenomenon can be well demonstrated with lollipop graphs. A lollipop graph Lo(p,t) is obtained by attaching a path of length t to a vertex of the complete graph  $K_p$ . As an example, the graph Lo(7,3) with  $\omega(G)=7$  is depicted in Fig.1. For graph Lo(7,3) the corresponding g(S) lower bounds are: 1.9, 3.4, 5.1, 6.1, 6.3, 6.2 as S increases from 0 to 5.



Figure 1: Lollipop graph Lo(7,3)

The bounds for  $M_2$  represented by Eq.(2) and in Corollary 2 are incomparable. However, the calculation of  $M_2$  is straightforward whereas the calculation of  $\omega(G)$  is NP-hard. Corollary 2 is more useful than Eq.(2) which is an upper bound for  $M_2$ . Moreover, Corollary 2 is a special case, with r=2, of the following theorem due to Nikiforov (Lemma 10 in [24]).

**Theorem 4.** For every r > 0 and every graph G:

$$f(r) = \frac{w_r^2}{w_r^2 - w_{2r}} \le \omega(G)$$

It can be observed that for many graphs f(r) < f(2) with r > 2. However for some graphs this series of lower bounds for  $\omega(G)$  increases as r increases. For example, for lollipop graph Lo(7,3) depicted in Fig.1 the lower bounds f(r) are 1.9, 3.4, 4.6, 5.2 and 5.3 as r increases from 1 to 5.

### 3. Variable Zagreb indices

Milicević and Nikolić [25] introduced and investigated applications of variable first and second Zagreb indices defined as follows:

$${}^{s}M_{1}(G) = \sum_{u \in V} d^{2s}(u)$$
 and  ${}^{s}M_{2}(G) = \sum_{u \in E} d^{s}(u)d^{s}(v)$ 

Clearly with S=1 these equate to the original Zagreb indices. Andova and Petruševski [26] proved that  ${}^{s}M_{1}/n \leq {}^{s}M_{2}/m$  for S  $\in [0,0.5]$ , and Ilić and Stevanović [12] have derived upper and lower bounds for the variable Zagreb indices. Liu and Gutman [27] verified that for any S  $\geq 1$ 

$${}^{s}M_{2}(G) = \sum_{uv \in E} d^{s}(u)d^{s}(v) \le \left(\sum_{uv \in E} d(u)d(v)\right)^{s} = M_{2}^{s}(G)$$

Based on the previous considerations, inequality (4) can be restated as follows

$${}^{s}M_{2}(G) \le \left\{{}^{s/2}M_{1}(G)\right\}^{2} \frac{(\omega-1)}{2\omega}$$
(5)

and Corollary 3 becomes:

$${}^{2}M_{2}(G) \le M_{1}^{2}(G) \frac{(\omega - 1)}{2\omega}$$
 (6)

Then, following the approach in Corollary 4, we can conclude that if G is a chemical graph, other than K<sub>5</sub>, then  ${}^{2}M_{2}(G) \le 0.375M_{1}^{2}(G)$ .

Theorem 5. Let G be a triangle-free graph. Then

$${}^{s}M_{2}(G) \leq \frac{1}{4} {{}^{s/2}M_{1}(G)}^{2} = \frac{1}{4} {{}^{s-1}(u) + d^{s-1}(v)}^{2}$$

with equality, for example, if  $G=P_2$  path or  $G=C_4$  cycle.

Proof. Because G is a triangle-free graph,  $\omega(G)=2$  holds. From Eq.(3) we have

$$\left(\sum_{u \in V} d^{s}(u)\right)^{2} \leq 2 \left(\left(\sum_{u \in V} d^{s}(u)\right)^{2} - 2\sum_{u \in E} d^{s}(u)d^{s}(v)\right) = 2 \left(\sum_{u \in V} d^{s}(u)\right)^{2} - {}^{s}M_{2}(G) * 4$$

Consider the transformation formula [28] represented by

$$\sum_{u \in V} \Phi(u) = \sum_{u v \in E} \left[ \frac{\Phi(u)}{d(u)} + \frac{\Phi(v)}{d(v)} \right]$$

where  $\Phi(u)$  is a positive continuous function defined on the vertex set V of G. Now, by using this transformation rule, from (4) the result can be obtained. It is easy to show that the equality holds if G=P<sub>2</sub> path or G=C<sub>4</sub> cycle.

## 4. Common lower and upper bounds for $\mu^2$ and $M_2(G)/m$

In [16] a common lower and upper bound is formulated for  $\mu$  and  $\sqrt{M_2/m}$ :

$$\frac{1}{m}\sum_{uv\in E}\sqrt{d(u)d(v)} \leq \left\{\mu, \sqrt{\frac{M_2}{m}}\right\} \leq \max_{uv\in E}\sqrt{d(u)d(v)}$$

Here, it will be shown that by using the Zagreb indices it is possible to establish novel sharp common lower and upper bounds for  $\mu$  and  $\sqrt{M_2/m}$ .

Hong [31] proved that for graphs with no isolated vertices

$$\mu^2(G) \le 2m - n + 1 \tag{7}$$

with equality if and only if G is a complete graph  $K_n$  or a star graph  $S_n$ . This suggests the following theorem.

Theorem 6. Let G be a graph with no isolated vertices. Then

$$M_{2}(G) \le m(2m - n + 1)$$
 (8)

with equality if G is a complete graph K<sub>n</sub> or a star graph S<sub>n</sub>.

Proof. Das and Gutman [8] proved that

$$M_{2}(G) \leq 2m^{2} - (n-1)m\delta + \frac{1}{2}(\delta - 1)m\left(\frac{2m}{n-1} + n - 2\right)$$
(9)

with equality if and only if G is isomorphic to Kn or Sn.

Simple algebra and the fact that  $2m \le n(n-1)$  verifies that

$$2m^{2} - (n-1)m\delta + \frac{1}{2}(\delta - 1)m\left(\frac{2m}{n-1} + n - 2\right) \le m(2m-n+1)$$
.

From (7) and(8) one obtains

$$\max\left\{\mu(G), \sqrt{M_2(G)/m}\right\} \le \sqrt{2m-n+1}$$

with equality if G is a complete graph K<sub>n</sub> or a star graph S<sub>n</sub>.

**Remark 1.** We can derive a novel upper bound for  $M_2$  which is stronger for some graphs than the Das and Gutman bound represented by (9): It is easy to verify that for a graph G with no isolated vertices:

$$M_{2}(G) \le m [2m - n + 1 - (\delta - 1)(n - 1 - \Delta)]$$
(10)

with equality, for example, if G is a regular graph or a star graph S<sub>n</sub>.

Proof. It is known that for the first and the second Zagreb indices the following relations are valid:

$$\mathbf{M}_1 = \sum_{\mathbf{u} \in \mathbf{V}} \mathbf{d}^2(\mathbf{u}) \le 2\mathbf{m}\Delta, \qquad \qquad 2\mathbf{M}_2 = \sum_{\mathbf{u} \in \mathbf{V}} \mathbf{d}^2(\mathbf{u})\mathbf{d}_{av}(\mathbf{u})$$

where  $d_{av}(u)$  is the average-degree of the vertices adjacent to a vertex u. Now, following the approach outlined in [8] we have that

$$d(u)d(u)_{av} \leq 2m - d(u) - (n - 1 - d(u))\delta.$$

This implies that

$$2M_{2} = \sum_{u \in V} d^{2}(u)d_{av}(u) \leq \sum_{u \in V} d(u) [2m - d(u) - (n - 1 - d(u))\delta] = 4m^{2} - 2m(n - 1)\delta + (\delta - 1)\sum_{u \in V} d^{2}(u)$$

Because

$$2M_{_2} \leq 4m^2 - 2m(n-1)\delta + (\delta-1)\sum_{u \in V} d^2(u) \leq 4m^2 - 2m(n-1)\delta + 2m(\delta-1)\Delta,$$

one obtains

$$M_{_2} \leq 2m^2 - m(n-1)\delta + m(\delta-1)\Delta = m \big[ 2m - n + 1 - (\delta-1)(n-1-\Delta) \big]. \tag{11}$$

The above inequality reduces to (8) if  $\delta = 1$ . It is easy to check that equality holds in (10) if G is a regular graph or a star graph  $S_n$ .

Remark 2. Das and Kumar [32] proved that

$$\mu^{2}(G) \leq 2m - (n-1)\delta + (\delta - 1)\Delta$$
(12)

and equality holds if and only if G is a regular graph or a star graph S<sub>n</sub>.

From inequalities (11) and (12) it can be concluded that

 $\mu^2(G) \le 2m - n + 1 - (\delta - 1)(n - 1 - \Delta),$ 

and equality is attained if G is a regular graph or a star graph S<sub>n</sub>.

As it is known [18, 9],  $\mu^2(G) \ge M_1(G)/n$  and  $\mu(G) \ge 2M_2(G)/M_1(G)$ . From the previous considerations it follows that

$$\max\left\{\sqrt{M_{1}(G)/n}, 2M_{2}(G)/M_{1}(G)\right\} \leq \max\left\{\!\mu(G), \sqrt{M_{2}(G)/m}\right\} \leq \sqrt{2m - n + 1 - (\delta - 1)(n - 1 - \Delta)} + \frac{1}{2} \left(\frac{1}{2}\right) \left(\frac{1}{2}\right$$

On the right-hand side, equality holds if and only if G is a regular graph or a star graph S<sub>n</sub>.

## 5. Answering a question due to Nikiforov

Nikiforov asks (Problem 7 in [24]) whether it is true that for connected bipartite graphs

$$\mu^{r}(G) \geq \frac{W_{q+r}(G)}{W_{q}(G)};$$

for every even  $q \ge 2$  and  $r \ge 2$ ?

Letting q=r=2 this inequality reduces to

$$\mu^2(\mathbf{G}) \ge \frac{\mathbf{w}_4(\mathbf{G})}{\mathbf{w}_2(\mathbf{G})} = \frac{\mathbf{M}_2}{\mathbf{m}} \cdot$$

Let  $C_k^3$  be the graph obtained by attaching 3 pendent vertices to each vertex of a cycle of length k. When  $k \ge 4$  is even this graph is connected and bipartite. It can be easily obtained that  $\mu(C_k^3) = 3$ ,  $m(C_k^3) = 4k$  and  $M_2(C_k^3) = 40k$ . This infinite set of unicyclic graphs therefore provides counter-examples. Furthermore, Nikiforov [24] proved that for r > 0 and odd q > 0

$$\mu^{r}(G) \ge \frac{W_{q+r}(G)}{W_{q}(G)}$$

Let q=3 and r=1, and we obtain a result due to Zhou [9] that  $M_2/M_1 \le \mu(G)/2$ . Reti [33] proved that  $M_2/M_1 \ge \delta/2$ . In both cases equality holds for regular graphs. If instead we let q=1 and r=3 then we reproduce the following bound due to Teranishi [17] that  $M_2 \le n\mu^3(G)/2$ , where equality is fulfilled if and only if G is a regular graph.

## 6. A series of approximations for $\mu(G)$

As already discussed, there are connected graphs for which  $\mu^2(G) \approx w_4(G)/w_2(G)$  is fulfilled. It is known that  $d^2(G) \leq M_1(G)/n \leq \mu^2(G)$ . Based on this observation it can be supposed that  $M_1(G)/n \approx d(G)\mu(G)$ . More exactly, we can suppose that there exists a particular class of connected graphs for which

$$\mu(G) \approx \frac{M_1(G)}{2m} = \frac{w_3(G)}{w_2(G)}.$$

It is easy to see that there are connected graphs satisfying the equality  $\mu(G)=w_3(G)/w_2(G)$ . Such graphs are shown in Fig.2. For these graphs  $\mu(H_A)=2$  and  $\mu(H_B)=3$ .



Figure 2: Graphs  $H_A$  and  $H_B$  satisfying the equality  $\mu(G)=w_3(G)/w_2(G)$ 

This suggests the following theorem, for which we first require a lemma that is due to Myerson [29].

**Lemma 1.** The number of k-walks of path  $P_4$  for  $k \ge 3$  is characterized by the following Fibonacci sequence:  $w_k = w_{k-1} + w_{k-2}$ .

Proof. Label the vertices A, B, C and D in order from left to right. Let  $a_k$  be the number of walks of length k starting at A, and similarly for  $b_k$ ,  $c_k$  and  $d_k$ .

Clearly,  $w_k = a_k + b_k + c_k + d_k$  and by symmetry  $a_k = d_k$  and  $b_k = c_k$ . Furthermore,  $a_k = b_{k-1}$ , because every path that starts at A must begin by going to B, and  $b_k = a_{k-1} + c_{k-1}$ , because every path that starts at B must start by going to either A or C. Therefore

$$\mathbf{b}_{k} = \mathbf{a}_{k-1} + \mathbf{c}_{k-1} = \mathbf{a}_{k-1} + \mathbf{b}_{k-1} = \mathbf{b}_{k-2} + \mathbf{b}_{k-1}$$
,

and similarly for  $a_k$ ,  $c_k$  and  $d_k$ .

**Theorem 7.** Let  $\Omega$  be the family of graphs with no isolated vertices. Then for even  $q \ge 2$  and  $r \ge 1$ :

$$\mu^{r}(G) \approx W_{r+q} / W_{q}$$
 if  $G \in \Omega$ .

Proof. Case 1: Graphs with  $\mu^{r}(G) = w_{r+q}/w_{q}$ .

For a connected regular graph G one obtains that  $w_k(G)=nd^{k-1}$ . Therefore,

$$\frac{w_{r+q}(G)}{w_{q}(G)} = \frac{nd^{r+q-1}}{nd^{q-1}} = \mu^{r}(G)$$

Case 2: Graphs with  $\mu^{r}(G) < w_{r+q}/w_{q}$ .

Let G=P<sub>4</sub> be a path for which  $\mu(P_4) = \varphi = (1 + \sqrt{5})/2 = 1.61803$  (the golden ratio). Clearly, w<sub>1</sub>=4 and w<sub>2</sub>=6. From Lemma 1, for  $r \ge 3$ , w<sub>k</sub> can be calculated as follows: w<sub>k</sub> = w<sub>k-1</sub> + w<sub>k-2</sub>. The number of k-walks in P<sub>4</sub> is therefore a Fibonacci sequence with initial values 4 and 6, and is the sequence A078642 in the On-line Encyclopedia of Integer Sequences (OEIS). As readers will be well aware, the original Fibonacci sequence are the numbers 1,1,2,3,5,8,13,21,...and the r-th term in this series is denoted by F(r). The OEIS states that the r-th term of sequence A078642 equals 2F(r+2).

Therefore, using the Binet's formula for F(r) with  $\psi = -1/\phi = -0.61803$ , one obtains that

$$w_{r} = \frac{2(\Phi^{r+2} - \Psi^{r+2})}{\sqrt{5}}$$

Hence, for even q

$$\frac{w_{r+q}}{w_q} = \frac{\Phi^{r+q+2} - \Psi^{r+q+2}}{\Phi^{q+2} - \Psi^{q+2}} > \Phi^r = \mu^r$$

Case 3: Graphs with  $\mu^{r}(G) > w_{r+q}/w_{q}$ .

Let G=P<sub>4</sub> U K<sub>2</sub>. Clearly, w<sub>1</sub>=6, w<sub>2</sub>=8 and  $\mu$ (G)= $\phi$ . Moreover, w<sub>k</sub>(K<sub>2</sub>)=2 for all k. Using the results discussed above, it follows that

$$w_r(G) = 2 + \frac{2(\Phi^{r+2} - \Psi^{r+2})}{\sqrt{5}}$$

We are therefore seeking to prove that for even q

$$\frac{w_{r+q}}{w_q} = \frac{\Phi^{r+q+2} - \Psi^{r+q+2} + \sqrt{5}}{\Phi^{q+2} - \Psi^{q+2} + \sqrt{5}} < \Phi^r = \mu^r$$

This simplifies to  $\Psi^{q+2}(\Phi^r - \Psi^r) < \sqrt{5}(\Phi^r - 1)$ , which is true for all r. By this the proof of Theorem 7 is completed.

We can investigate this theorem experimentally. It is well known (see, for example, Lemma 2.5 in [1]) that the number of walks of length r+1 in G, from  $v_i$  to  $v_j$ , is the entry  $a^{(r)}(i,j)$  in position (i,j) of the matrix  $A^r$ .

Consequently,

$$w_{r+1} = w_{r+1}(G) = j^{T}A^{r}j = \sum_{\{i,j\}} a_{i,j}^{(r)}$$

It should be noted that we have followed Nikiforov [24] in measuring the length of a walk by the number of vertices from beginning to end, whereas Biggs [1] measures the length of a walk by the number of edges from beginning to end. This explains the apparent discrepancy between our formula for  $w_k$  and Lemma 2.5 in [1].

We selected the 59 named graphs on 10 vertices in Wolfram Mathematica to assess how well the spectral radius approximations by means of the number of walks perform. Using increasing values of r, we have compared the spectral radii  $\mu(G)$  of these graphs with the estimated spectral radii  $\mu_A$  calculated by

$$\mu_{A} \cong \sqrt[r]{\frac{w_{r+2}(G)}{w_{2}(G)}} = \sqrt[r]{\frac{w_{r+2}(G)}{2m}}$$

Evaluating the computed results obtained in the considered cases, the following conclusion can be drawn: If r increases from 1 to 5, the accuracy of the approximation to  $\mu$  (i.e. the relative deviation between the values  $\mu$ (G) and  $\mu$ <sub>A</sub>) is on average 2% too high, 0.35% too low, 0.3% too high, 0.2% too low and 0.1% too high.

Nikiforov [24] has observed that if G is connected and non-bipartite, then  $w_{r+q}/w_q$  tends to  $\mu^r(G)$  as q tends to infinity. Moreover, it has been demonstrated [24] that for bipartite graphs, if q is even and r is odd,  $\mu^r(G)$  can differ considerably from  $w_{r+q}/w_q$ , no matter how large q is.

## 7. The case of equality

A connected graph with an adjacency matrix A=A(G) is called [16,41]:

-semiharmonic if  $A^3j = \mu^2 Aj$ ,

-harmonic (or pseudoregular) if  $A^2 j = \mu A j$ ,

-semiregular, if it is bipartite and  $A^2 j = \mu^2 j$ ,

-pseudo-semiregular if it is bipartite and vertices belonging to the same part of bipartition have the same average degree [16, 30].

From these definitions it follows that all regular graphs are harmonic, and moreover, the harmonic, semiregular, and pseudo-semiregular graphs form subsets of semiharmonic graphs.

Let q and r be positive integers, and denote by  $Z_{r,q}$  the set of graphs for which  $\mu^r = w_{r+q}/w_q$  holds. To characterize or classify the connected  $Z_{r,q}$  graphs is a complicated problem. It seems unlikely that it is possible to identify every graph for which  $\mu^r = w_{r+q}/w_q$ . It is known that set  $Z_{1,2}$  contains acyclic and cyclic graphs. (See graphs depicted in Fig.2.)

Recently, it has been verified [16] that the set  $Z_{2,2}$  includes regular and semiharmonic graphs. In [16], it is also demonstrated that the set  $Z_{2,2}$  contains so-called "sporadic graphs" which do not belong to the family of semiharmonic graphs.

As an example, in Fig.3 a bipartite and a non-bipartite graph belonging to set  $Z_{2,2}$  are depicted. They are sporadic, because they are not semiharmonic. For these graphs  $\mu(J_A)=\sqrt{5}$  and  $\mu(J_B)=3$ .



Figure 3: A bipartite graph (J<sub>A</sub>) and a non-bipartite graph (J<sub>B</sub>) belonging to set Z<sub>2,2</sub>

**Theorem 8.** Let G be a connected graph with a spectral radius  $\mu(G)$ . If  $\mu^r = w_{r+q}/w_q$  holds for certain q>0 and r >0, then  $\mu^r$  is an integer.

Proof. The characteristic polynomial of G is a monic polynomial with integer coefficients. Consequently,  $\mu(G)$  and  $\mu^{r}(G)$  are algebraic integers. Furthermore  $w_{r+q} / w_{q}$  is a rational number. It is known that the only algebraic integers in the set of rational numbers are integers. Therefore  $\mu^{r}(G)$  is an integer and  $w_{r+q}$  is divisible by  $w_{q}$ .

The relevant results concerning the relations between the walk numbers and the spectral radius of graphs are summarized in [24, 41, 42, 43].

It is worth noting that in [30] the following theorem was proved: If G is a connected graph, then

$$\mu^{2}(G) \geq \frac{w_{5}(G)}{w_{3}(G)} = \frac{\sum_{u \in V} D_{2}^{2}(u)}{\sum_{u \in V} d^{2}(u)} = \frac{\sum_{u \in V} [d(u)d_{av}(u)]^{2}}{M_{1}(G)}$$

with equality if and only if G is a harmonic or a bipartite pseudo-semiregular graph.

Using a spectral approach, Nikiforov verified that harmonic graphs belong to the family of  $Z_{r,q}$  graphs. In what follows we present a simple alternative proof based on elementary graph theoretical considerations.

**Theorem 9.** Let G be a harmonic graph with a spectral radius  $\mu(G)$ . Then for arbitrary  $r \ge 1$  and  $q \ge 2$  we have:

$$\mu^{r}(G) = \frac{W_{r+q}(G)}{W_{q}(G)}$$

Proof. Because for a harmonic graph G, the equality  $A^2j = \mu Aj$  holds, it follows on the one hand, that

$$A^{r}j = A^{r-1}(Aj) = \mu^{r-1}Aj$$

on the other hand,

$$W_{r+1}(G) = j^{T}A^{r}j = \mu^{r-1}j^{T}Aj = 2m\mu^{r-1}.$$

This implies that if  $r \ge 2$  then

 $W_r(G) = 2m\mu^{r-2}$ 

Consequently, for arbitrary  $r \ge 1$  and  $q \ge 2$  integers one obtains:

$$\frac{w_{r+q}(G)}{w_{q}(G)} = \frac{2m\mu^{r+q-2}}{2m\mu^{q-2}} = \mu^{r}(G)$$

Corollary 6. If G is a harmonic graph then

$$\mu(G) = \frac{M_1(G)}{2m} = \frac{2M_2(G)}{M_1(G)} = \sqrt{\frac{M_2(G)}{m}} \cdot$$

**Corollary 7.** Let  $r \ge 1$  and  $q \ge 2$  be arbitrary integers. There exist infinite subsets of bipartite and non-bipartite  $Z_{r,q}$  graphs characterized by an identical spectral radius, and for these graphs  $\mu^r = w_{r+q}/w_q$  holds.

In Fig.4 infinite sequences of harmonic graph pairs denoted by  $G_A(k)$  and  $G_B(k)$  are shown. These graphs can be bipartite and non-bipartite, and they have identical spectral radius  $\mu(G_A(k))=\mu(G_B(k))=3$  for any  $k\geq 3$  integer.



Figure 4: Infinite sequences of harmonic graphs  $G_A(k)$  and  $G_B(k)$  (case of k=5)

For graphs  $G_A(k)$  and  $G_B(k)$  the equalities m=4k, and m<sub>22</sub>=k, m<sub>24</sub>=2k, m<sub>44</sub>=k hold, where quantities m<sub>pq</sub> denote the numbers of edges in a graph with end-vertices of degree p and q. This implies that  $G_A(k)$  and  $G_B(k)$  are characterized by identical vertex-degree based topological indices.

Complete bipartite graphs represent a subset of semiregular graphs. The proof of the following theorem is based on the concept outlined in [24].

**Theorem 10.** Let  $K_{a,b}$  be a complete bipartite graph with  $1 \le a < b$  positive integers. If  $r \ge 2$  even, then  $\mu^r = w_{r+q}/w_q$  holds where  $\mu(K_{a,b}) = \sqrt{ab}$ .

Proof. For a complete bipartite graph  $K_{a,b}$  the corresponding spectral radius is equal to  $\sqrt{ab}$  [30]. According to Nikiforov [24], it is known that for  $k \ge 1$  and  $j \ge 1$  integers

$$w_{2k}(K_{a,b}) = 2(ab)^k$$
  
 $w_{2k+i}(K_{a,b}) = (a+b)(ab)^{k+(j-1)/2}$ 

Considering the values of  $w_{r+q}/w_q$ , it is obvious that r will be even only in two cases: (i) if q is even and r+q is even, or (ii) q is odd and r+q is odd.

CASE (i): Let  $k \ge 1$  and  $p \ge 1$  be arbitrary integers. Because q=2k and r=2p are even numbers, consequently,

$$W_{r+q}(K_{a,b}) = W_{2(k+p)} = 2(ab)^{k+p}$$
.

It follows that

$$\frac{w_{r+q}(K_{a,b})}{w_{q}(K_{a,b})} = \frac{w_{2(k+p)}}{w_{2k}} = \frac{2(ab)^{k+p}}{2(ab)^{k}} = (ab)^{p} = (ab)^{r/2} = \mu^{r}(G),$$

CASE (ii): Let r=2p, where  $p \ge 1$  integer. Because r is even, q and r+q are odd, this implies that

$$w_{q}(K_{a,b}) = w_{2k+j}$$
 and  $w_{r+q}(K_{a,b}) = w_{2(k+p)+j}$ 

It follows that

$$\frac{w_{r+q}(K_{a,b})}{w_a(K_{a,b})} = \frac{w_{2(k+p)+j}}{w_{2k+j}} = \frac{(a+b)(ab)^{k+p+(j-1)/2}}{(a+b)(ab)^{k+(j-1)/2}} = (ab)^p = (ab)^{r/2} = \mu^r(G)$$

### 8. Final remarks and conclusions

Zagreb indices have numerous applications in mathematical chemistry. In this paper we have used results from spectral graph theory, including the number of open walks in graphs, to suggest results primarily for the Zagreb indices.

Nikiforov [24] proved that for odd q,  $w_{r+q}/w_q \le \mu^r(G)$  holds, and identified all families of graphs for which there is equality. In this paper we have proved that for even q,  $w_{q+r}/w_q \approx \mu^r$  is fulfilled. Additionally, as an example, we have presented various sporadic graphs for which equality holds. This finding implies that it would be very hard to identify all graphs for which there is equality with even q.

It should be emphasized that there is a strong correspondence between Zagreb indices and the walk numbers in a graphs.

For example, the well-known Zagreb indices inequality [11, 12, 15, 34-38] can be rewritten in the following alternative form:

$$Z(G) = \frac{M_2(G)}{m} - \frac{M_1(G)}{n} = \frac{1}{w_1w_2}(w_1w_4 - w_2w_3) \ge 0$$

It has been verified that the Zagreb indices inequality  $(Z(G) \ge 0)$  is true for a broad class of connected graphs: for chemical graphs with maximum degree four, bidegreed graphs, acyclic graphs, unicyclic graphs, threshold graphs, graphs with vertex degrees in any interval of length three [11, 12, 15, 34-38]. The bound is sharp and for example, the equality  $w_1w_4$ - $w_2w_3$ =0 holds if G is a regular or semiregular graph [36, 37].

Moreover, it was also demonstrated that there are infinitely many connected graphs, that are neither regular nor semiregular, which satisfy the Zagreb indices equality [39]. The Zagreb indices inequality is not valid for general graphs. For example, counter examples can be constructed for connected bicyclic and tricyclic graphs [37, 40]. From these considerations it follows that for the family of connected graphs  $w_4/w_2 \approx w_3/w_1$  holds.

Täubig et al. [42,43] have proved that if  $k \ge 2$ ,  $l \ge 0$  and  $p \ge 0$  are integers, then

$$w_{2l+p+1}^{k} \le w_{2l+1}^{k-1} w_{2l+pk+1}.$$
(13)

The above formula represents a generalization of the two sharp inequalities for Zagreb indices, published by Ilić and Stevanović [12]. As particular cases, from (13) we obtain directly the following equivalent inequalities:

- a) if k=2, l=0 and p=1 then
  - $w_2^2 \le w_1 w_3$  and  $\frac{M_1(G)}{n} \ge \frac{4m^2}{n^2}$ ,
- b) if k=3, l=0 and p=1 then

$$w_2^3 \leq w_1^2 w_4 \qquad \qquad \text{and} \qquad \qquad \frac{M_2(G)}{m} \geq \frac{4m^2}{n^2} \,.$$

We have noted that  $M_1(G)=w_3$  and  $M_2(G)=w_4/2$ . It may therefore be of interest to "define higher Zagreb indices" such as  $M_3(G)=w_5/3=(j^TA^4j)/3$  and  $M_4(G)=w_6/4=(j^TA^5j)/4$ . It would be worth testing whether these higher Zagreb indices possess any practical applicability in mathematical chemistry. Performing such tests, the explanatory, discriminatory and predictive powers of these higher Zagreb indices could then be compared with that for the traditional degree-based topological indices.

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