MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 689-698

ISSN 0340 - 6253

New sharp upper bounds for the first Zagreb index*

Muhuo Liu[1,2], Bolian Liu[2]

[1] Department of Applied Mathematics, South China Agricultural University, Guangzhou, P. R. China, 510642

[2] School of Mathematic Science, South China Normal University, Guangzhou, P. R. China, 510631

(Received October 15, 2008)

Abstract: This paper presents some new upper bounds for the first Zagreb index.

1 Introduction

In this paper, we only consider connected simple graphs and in the remainder of the text by term graph we should imply connected simple graph. Let $G = (V, E)$ be a graph with $|V| = n$ and $|E| = m$. Sometimes we refer to G as an (n, m) graph. The symbol uv is used to denote an edge, whose endpoints are the vertices u and v. Let $N(u)$ be the first neighbor vertex set of u, then $d(u) = |N(u)|$ is called the degree of u. Specially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are called the maximum and minimum degree of vertices of G, respectively. As usual, K_n, $K_{1,n-1}$ and C_n denote a complete graph, a star and a cycle of order n, respectively.

Let $A(G)$ be the adjacency matrix of G and $D(G) = diag(d(v_1), d(v_2), ..., d(v_n))$ the diagonal matrix of vertex degrees of G. The *Laplacian matrix* of G is $L(G) = D(G) - A(G)$ and the *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$. If B is a real symmetric

*The first author is supported by the fund of South China Agricultural University (No. 2008K012); The second author is the corresponding author who is supported by NNSF of China (No. 10771080) and SRFDP of China (No. 20070574006). E-mail address: liubl@scnu.edu.cn

matrix, it is well known that the eigenvalues of B are real numbers. Thus, we can use $\rho(B)$ to denote the greatest eigenvalue of B.

The Zagreb indices were first introduced by Gutman and Trinajstić [1], they are important molecular descriptors and have been closely correlated with many chemical properties [2]. Thus, they attract more and more attention from chemists and mathematicians [3–12]. The *first Zagreb index* $M_1 = M_1(G)$ is defined as:

$$M_1(G) = \sum_{v \in V} d(v)^2.$$

In this paper, we obtain some new sharp upper bounds for M_1.

2 Some new upper bounds for M_1

Up to now, some upper bounds for M_1 in term of m, n, Δ and δ have been obtained:

Theorem A [**3**]**:** Let G be a connected (n, m) graph. Then

$$M_1 \leq m(m+1), \tag{1}$$

with equality attained, for example, by $K_{1,n-1}$ and K_3.

Theorem B [**4**]**:** Let G be a connected (n, m) graph. Then

$$M_1 \leq n(2m - n + 1), \tag{2}$$

with equality holding if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Theorem C [5]**:** Let G be a connected (n, m) graph. Then

$$M_1 \leq m\left(\frac{2m}{n-1} + n - 2\right), \tag{3}$$

with equality holding if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Theorem D [**6**]**:** Let G be a connected (n, m) graph. Then

$$M_1 \leq m\left(\frac{2m}{n-1} + \frac{n-2}{n-1}\Delta + (\Delta - \delta)(1 - \frac{\Delta}{n-1})\right), \tag{4}$$

with equality holding if and only if G is a star graph or a regular graph.

Remark 1. It is easy to see that $m(\frac{2m}{n-1} + \frac{n-2}{n-1}\Delta + (\Delta - \delta)(1 - \frac{\Delta}{n-1})) \leq m(\frac{2m}{n-1} + n - 2)$ (for details see [6], p. 64). Thus, the bound (4) is always better than (3).

Remark 2. If G is a connected (n, m) graph, then $m \leq \frac{n(n-1)}{2}$. This implies that

$m(\frac{2m}{n-1}+n-2) = mn+2m(\frac{m}{n-1}-1) \leq mn+n(n-1)(\frac{m}{n-1}-1) = n(2m-n+1)$. Thus, the bound (3) is usually finer than (2).

Remark 3. If $m = n-1$, then the bound (2) is equal to (1). If $m \geq n$, let us prove that $m(m+1) \geq n(2m-n+1)$. We only need to prove that $m^2-2mn+m+n(n-1) \geq 0$. Let $f(x) = x^2-2xn+x+n(n-1)$, where $x \geq n$. When $x \geq n$, since $f'(x) = 2x-2n+1 > 0$, then $f(x) \geq f(n) = 0$. Thus, the bound (2) is usually lower than (1).

For the symmetric matrix, it is well known that

Lemma 2.1 [13] *Suppose $B = B_{n\times n}$ is a symmetric nonnegative irreducible matrix with row sums $s_1, s_2, ..., s_n$, then*

$$\min_{1\leq i\leq n} s_i \leq \rho(B) \leq \max_{1\leq i\leq n} s_i.$$

Moreover, one of the equalities holds if and only if the row sums of B are all equal.

Lemma 2.2 [14] (*Rayleigh-Ritz Theorem*) *Suppose $B = B_{n\times n}$ is a symmetric matrix, then*

$$\rho(B) \geq \frac{x^T Bx}{x^T x},$$

where $x(\neq 0)$ is a n-tuple column-vector. Moreover, if the equality holds, then x is an eigenvector corresponding to $\rho(B)$.

Lemma 2.3 [6] *Let G be a connected graph and $D_{uv} = \{d(u)+d(v) : uv \in E(G)\}$. Then all D_{uv} are equal if and only if G is a regular graph or a bipartite semiregular graph.*

Let $K(G)$ denote the adjacency matrix of the line graph of G, $C = C(G)$ denote the incidence matrix of G, it is readily to check that $Q(G) = A(G) + D(G) = CC^T$ and $C^T C = K(G) + 2I$ (see [15],p23).

Theorem 2.1 *Let G be a connected (n, m) graph. Then*

$$M_1 \leq m\rho(Q(G)), \tag{5}$$

the equality holds if and only if G is a regular graph or a bipartite semiregular graph.

Proof. In the proof of this theorem, let $F = C^T C = K(G)+2I$. Recall that $Q(G) = CC^T$ and $C^T C$ share common non-zero eigenvalues, then $\rho(Q(G)) = \rho(F)$. Let $x = (1, 1, ..., 1)^T$, namely, x is a m-tuple column-vector with every entry is 1. Lemma 2.2 implies that

$$\rho(Q(G))=\rho(F)\geq\frac{x^TFx}{x^Tx}=\frac{\sum_{uv\in E}(d(u)+d(v))}{m}=\frac{\sum_{v\in V}d(v)^2}{m}=\frac{M_1}{m},$$

thus the required inequality (5) follows.

If the equality holds, by Lemma 2.2, $x=(1,1,...,1)^T$ is an eigenvector corresponding to $\rho(F)$. Thus, $d(u)+d(v)=\rho(F)$ holds for all $uv\in E(G)$. By Lemma 2.3, it follows that G is a regular graph or a bipartite semiregular graph. Conversely, if G is a regular graph or a bipartite semiregular graph, then $d(u)+d(v)=k$ holds for any $uv\in E$ by Lemma 2.3. Combining with Lemma 2.1, it follows that $\rho(F)=k$. Thus, $M_1=\sum_{v\in V}d(v)^2=\sum_{uv\in E}(d(u)+d(v))=mk=m\rho(Q(G))$, i.e., the equality holds.

In [17], Anderson and Morley proved that

Lemma 2.4 [17] $\rho(Q)\leq max\{d(u)+d(v):uv\in E\}$.

Note that if G is a triangle-free (n,m) graph, then $d(u)+d(v)=|N(u)\cup N(v)|\leq n$ holds for every $uv\in E$. Thus, Theorem 2.1 and Lemma 2.4 imply that

Corollary 2.1 [4] *If G is a connected triangle-free (n,m) graph, then $M_1\leq mn$.*

Remark 4. By combining the results in [6,16], we have $\rho(Q(G))\leq\max\{d(v)+m(v):v\in V\}\leq\frac{2m}{n-1}+\frac{n-2}{n-1}\Delta+(\Delta-\delta)\left(1-\frac{\Delta}{n-1}\right)$, where $m(v)=\sum\limits_{u\in N(v)}d(u)/d(v)$. Thus, by Theorem 2.1 it follows that

$$M_1\leq m\rho(Q(G))\leq m\left[\frac{2m}{n-1}+\frac{n-2}{n-1}\Delta+(\Delta-\delta)\left(1-\frac{\Delta}{n-1}\right)\right].$$

Remarks 1-3 imply that the bound (5) is always finer than bounds (1)-(4).

Lemma 2.5 [18] *Let G be a connected (n,m) graph. Then* $\rho(Q(G))\leq\max\{\Delta+\delta-1+\frac{2m-\delta(n-1)}{\Delta},\delta+1+\frac{2m-\delta(n-1)}{2}\}$.

By Theorem 2.1 and Lemma 2.5, it follows that

Theorem 2.2 *Let G be a connected (n,m) graph. Then*

$$M_1\leq\max\left\{m\left(\Delta+\delta-1+\frac{2m-\delta(n-1)}{\Delta}\right),m\left(\delta+1+\frac{2m-\delta(n-1)}{2}\right)\right\}\qquad(6)$$

equality can be obtained, for example, by a star or a regular graph of order $n\geq3$.

Corollary 2.2 *Let G be a connected (n,m) graph. If $\Delta \geq \frac{2m-\delta(n-1)}{2}$, then*

$$M_1 \leq m(\Delta+\delta+1).$$

Remark 5. Let $f(x) = x+\delta-1+\frac{2m-\delta(n-1)}{x}$, where $2 \leq x \leq n-1$. Since $f'(x) = 1-\frac{2m-\delta(n-1)}{x^2}$, thus $f(x) = x+\delta-1+\frac{2m-\delta(n-1)}{x} \leq \max\{n-2+\frac{2m}{n-1}, \delta+1+\frac{2m-\delta(n-1)}{2}\}$ because $2 \leq x \leq n-1$. When $n \geq 3$, since $\max\{m(n-2+\frac{2m}{n-1}), m(\delta+1+\frac{2m-\delta(n-1)}{2})\} \leq m(m+1)$, thus the bound (6) is better than (1) when $n \geq 3$.

Let $\mathbb{G}^*(m,n,\frac{2m-(n-1)}{2},1)$ be the classes of graphs with $\Delta \geq \frac{2m-(n-1)}{2}$, $m \geq n$ and $\delta = 1$. Next let us show that the bound (6) is better than bounds (2)-(4) in $\mathbb{G}^*(m,n,\frac{2m-(n-1)}{2},1)$.

By Remarks 1-2, We only need to prove that the bound (6) is better than (4) in $\mathbb{G}^*(m,n,\frac{2m-(n-1)}{2},1)$. When $\Delta = n-1$, since $\delta = 1$, it is clear that bound (6) is equal to (4). Thus, we only need to show that $\frac{2m}{n-1}+\frac{n-2}{n-1}\Delta+(\Delta-1)(1-\frac{\Delta}{n-1}) \geq \Delta+\frac{2m-(n-1)}{\Delta}$ when $\frac{n+1}{2} \leq \Delta \leq n-2$. Next we shall prove that $2\Delta-\frac{\Delta^2}{n-1}+\frac{2m}{n-1}-1 \geq \Delta+2$ when $\frac{n+1}{2} \leq \Delta \leq n-2$. Equivalently, we shall show that $(\Delta-3)(n-1)+2m-\Delta^2 \geq 0$ when $\frac{n+1}{2} \leq \Delta \leq n-2$. Once this is proved, we are done.

Let $f(x) = (x-3)(n-1)+2m-x^2$, where $\frac{n+1}{2} \leq x \leq n-2$. When $\frac{n+1}{2} \leq x \leq n-2$, since $f'(x) = n-1-2x$, then $f'(x) < 0$. Thus, $f(x) \geq f(n-2) = 2m+1-2n > 0$. This implies that $(\Delta-3)(n-1)+2m-\Delta^2 > 0$ holds when $\frac{n+1}{2} \leq \Delta \leq n-2$.

By combining the above arguments, we can conclude that

Remark 6. The bound (6) is better than bounds (2)-(4) in $\mathbb{G}^*(m,n,\frac{2m-(n-1)}{2},1)$.

In the following, we shall give another new bound for M_1 in term of m, n, Δ and δ. The next famous inequality is needed:

Lemma 2.6 (*Pólya-Szegő inequality*) *Let $0 < m_1 \leq a_k \leq M_1$, $0 < m_2 \leq b_k \leq M_2$ $(k = 1,2,...,n)$. Then*

$$\left(\sum_{k=1}^{n} a_k^2\right)\left(\sum_{k=1}^{n} b_k^2\right) \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}}+\sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2\left(\sum_{k=1}^{n} a_kb_k\right)^2$$

where the equality holds if and only if $a_1 = a_2 = \cdots = a_n$, $b_1 = b_2 = \cdots = b_n$.

Theorem 2.3 *Let G be a connected (n,m) graph. Then*

$$M_1 \leq \frac{(\Delta+\delta)^2}{n\Delta\delta}m^2, \tag{7}$$

equality holds if and only if G is regular.

Proof. Let $a_i = d(v_i)$ and $b_i = 1$ for $1 \le i \le n$, it is easy to see that $0 < \delta \le a_i \le \Delta$, and $0 < 1 \le b_i \le 1$. By Lemma 2.6 it follows that

$$M_1 \le \frac{1}{4n}\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 (2m)^2 = \frac{(\Delta+\delta)^2}{n\Delta\delta} m^2 .$$

Thus, inequality (7) follows.

If G is regular, it is easy to see that the equality holds. On converse, if the equality holds, by Lemma 2.6 it follows that $d(v_1) = d(v_2) = \cdots = d(v_n)$, then G is regular.

Corollary 2.3 *Let G be a connected (n, m) graph.* (1) *If $\delta = 1$, then $M_1 \le \frac{nm^2}{n-1}$. The equality holds if and only if $G \cong K_2$.* (2) *If $\delta \ge 2$, then $M_1 \le \frac{(n+1)^2}{2n(n-1)} m^2$. The equality holds if and only if $G \cong C_3$.*

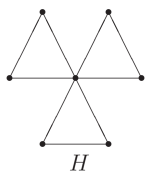
Proof. Let $f(x) = x + \frac{1}{x}$. Obviously, $f(x)$ is an increasing function for $x \ge 1$.

(1) If $\delta = 1$, note that $\frac{(\Delta+\delta)^2}{\Delta\delta} = \frac{\Delta}{\delta} + \frac{\delta}{\Delta} + 2$ and $1 \le \frac{\Delta}{\delta} = \Delta \le n-1$, by Theorem 2.3 $M_1 \le \frac{nm^2}{n-1}$. If $G \cong K_2$, it is readily to check that $M_1 = \frac{nm^2}{n-1}$. On converse, if $M_1 = \frac{nm^2}{n-1}$, then $n - 1 = \frac{\Delta}{\delta} = 1$ follows from Theorem 2.3, thus $G \cong K_2$.

(2) If $\delta \ge 2$, note that $1 \le \frac{\Delta}{\delta} \le \frac{n-1}{2}$, then $\frac{\Delta}{\delta} + \frac{\delta}{\Delta} + 2 \le \frac{(n+1)^2}{2(n-1)}$. If $G \cong C_3$, it is readily to check that $M_1 = \frac{(n+1)^2}{2n(n-1)} m^2$. On converse, if $M_1 = \frac{(n+1)^2}{2n(n-1)} m^2$, then $\frac{n-1}{2} = \frac{\Delta}{\delta} = 1$ follows from Theorem 2.3, thus $G \cong C_3$.

As shown in the next example, sometimes the bound (7) is better than (1), ..., (6). Thus, (7) is significative as a new bound.

Example 2.1 *Let H be the graph as shown in Fig. 1. The values of M_1 and of the bounds* (1)-(7) *for the graph H are also given in Fig. 1. Then for H, the bound* (7) *is better than* (1), ..., (6), *respectively.*



	M_1	(1)	(2)	(3)	(4)	(5)	(6)	(7)
H	60	90	84	72	72	66.35	72	61.71

Fig. 1.

3 The application of the bound (6)

In this section, with the help of the bound (6), we shall determine the first three (resp. four) largest M_1 in the classes of connected unicyclic graphs (resp. trees).

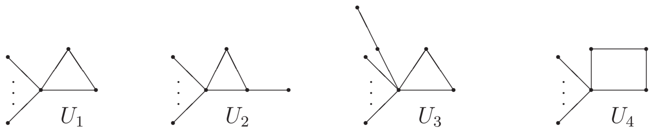


Fig. 2. The all connected unicyclic graphs with $\delta = 1$ and $\Delta \geq n-2$.

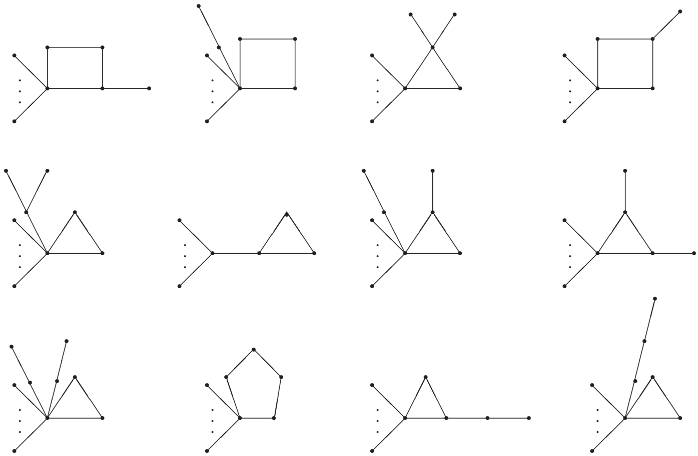


Fig. 3. The all connected unicyclic graphs with $\delta = 1$ and $\Delta = n-3$.

Let $\mathbb{U}(n)$ denote the classes of connected unicyclic graphs of order n. Let U_1, U_2, U_3, U_4 be the unicyclic graphs as shown in Fig. 2.

Theorem 3.1 *Let $G \in \mathbb{U}(n)$, if $n \geq 9$ and $G \in \mathbb{U}(n) \setminus \{U_1, U_2, U_3, U_4\}$, then $M_1(U_1) > M_1(U_2) > M_1(U_3) = M_1(U_4) > M_1(G)$.*

Proof. It is easy to see that $M_1(U_1) = n^2 - n + 6$, $M_1(U_2) = n^2 - 3n + 14$ and $M_1(U_3) = M_1(U_4) = n^2 - 3n + 12$. Next we shall prove that $M_1(G) < n^2 - 3n + 12$.

If $\delta \geq 2$, then G is a cycle. Thus, $M_1(G) = 4n < n^2 - 3n + 12$ follows.

If $\delta = 1$ and $\Delta \leq n-4$, by the bound (6) it follows that

$$M_1(G) \leq \max\left\{n\left(n-4+\frac{n+1}{n-4}\right),\, n\left(2+\frac{n+1}{2}\right)\right\} < n^2-3n+12\ .$$

If $\delta = 1$ and $\Delta = n-3$, note that there are only twelve connected unicyclic graphs with $\delta = 1$ and $\Delta = n-3$ (see Fig. 3), it is easily to check that $M_1(G) < n^2 - 3n + 12$ also follows.

Since U_1, U_2, U_3 and U_4 are the all connected unicyclic graphs with $\delta = 1$ and $\Delta \geq n-2$, then the conclusion follows by combining the above discussion.

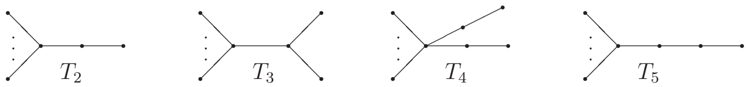


Fig. 4. The all trees with $n-3 \leq \Delta \leq n-2$.

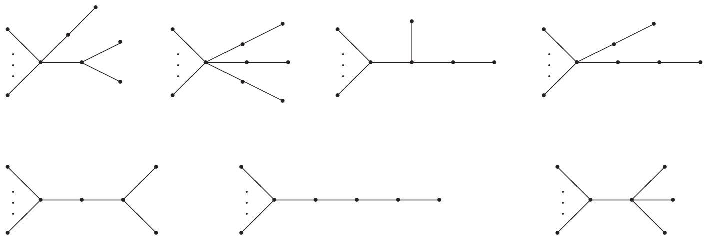


Fig. 5. The all trees with $\Delta = n-4$.

Let $\mathbb{T}(n)$ denote the classes of trees of order n. Let T_2, T_3, T_4 and T_5 be the trees as shown in Fig. 4.

Theorem 3.2 *Suppose that $T_1 \cong K_{1,n-1}$ and that $T \in \mathbb{T}(n)$. If $n \geq 9$ and $T \in \mathbb{T}(n) \setminus \{T_1, T_2, T_3, T_4, T_5\}$, then $M_1(T_1) > M_1(T_2) > M_1(T_3) > M_1(T_4) = M_1(T_5) > M_1(T)$.*

Proof. It is easy to see that $M_1(T_1) = n^2-n$, $M_1(T_2) = n^2-3n+6$, $M_1(T_3) = n^2-5n+16$ and $M_1(T_4) = M_1(T_5) = n^2-5n+14$. Next we shall prove that $M_1(T) < n^2-5n+14$.

If $\Delta \leq n-5$, by the bound (6) it follows that

$$M_1(T) \leq \max\left\{(n-1)\left(n-5+\frac{n-1}{n-5}\right),\, (n-1)\left(2+\frac{n-1}{2}\right)\right\} < n^2-5n+14\ .$$

If $\Delta = n-4$, note that there are only seven trees with $\Delta = n-4$ (see Fig. 5), it can be easily checked that $M_1(T) < n^2 - 5n + 14$ also follows.

Since T_1, T_2, T_3, T_4 and T_5 are the all trees with $\Delta \geq n-3$, then the conclusion follows by combining the above discussion.

Acknowledgements

The authors are grateful to the referees for their valuable comments, corrections and suggestions, which lead to an improvement of the original manuscript.

References

[1] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi-$electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[2] X. L. Li, I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, Univ. Kragujevac, Kragujevac, 2006.

[3] K. C. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujevac J. Math.* **25** (2003) 31–49.

[4] B. Zhou, Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 113–118.

[5] D. de Caen, An upper bound on the sum of squares of degrees in a graph, *Discr. Math.* **185** (1998) 245–248.

[6] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, *Discr. Math.* **285** (2004) 57–66.

[7] B. L. Liu, I. Gutman, Upper bounds for Zagreb indices of connected graphs, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 439–446.

[8] B. Zhou, Remarks on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 591–596.

[9] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[10] B. Liu, I. Gutman, Estimating the Zagreb and the general Randić indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 617–632.

[11] F. Xia, S. Chen, Ordering unicyclic graphs with respect to Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 663–673.

[12] H. Hua, Zagreb M_1 index, independence number and connectivity in graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 45–56.

[13] H. Minc, *Nonegative Matrices*, Wiley, New York, 1988 (Chapter 2).

[14] R. A. Horn, C. R. Johnson, *Matrix Analysis*, Cambridge Univ. Press, Cambridge, 1985.

[15] B. L. Liu, *Combinatorial Matrix Theory* (in Chinese), Science Press, Beijing, 2005.

[16] K. C. Das, The Laplacian spectrum of a graph, *Computers Math. Appl.* **48** (2004) 715–724.

[17] W. N. Anderson, T. D. Morley, Eigenvalues of the Laplacian matrix of a graph, *Lin. Multilin. Algebra* **18** (1985) 141–145.

[18] F. Y. Wei, M. H. Liu, A sharp upper bound on the Laplacian and signless Laplacian spectral radius of a graph, *Lin. Algebra Appl.*, submitted.