Advanced Studies in Contemporary Mathematics
31 (2021), No. 1, pp. 49 - 66

www.jangjeon.or.kr
http://dx.doi.org/10.17777/ascm2021.31.1.49

MAXIMUM DEGREE ENERGY

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Abstract. In this paper, maximum degree energy of graphs is studied. After giving some preliminary new results, bounds for the maximum degree eigenvalues are obtained for a general graph. Also bounds on the maximum degree eigenvalues of some frequently used graph classes are given by means of combinatorial, number theoretical and analysis methods. Many proofs are established by means of some result obtained by Adiga and Smitha. Maximum degree energy is calculated for any given simple graph and also for some classes of graphs and obtained relations with others. Special emphasis is given to unicyclic graphs. Several unicyclic graph classes are defined and their maximum degree eigenvalues and energy are calculated.

2010 Mathematics Subject Classification. 05C07, 05C30, 05C38, 05C76.

Keywords and phrases. Harmonious coloring, harmonious chromatic number, lexicographic product.

1. Introduction

The graph energy is one of the most important graph invariants in chemical graph theory. It was originally inspired [1] by the Hückel molecular orbital approximation, where it relates to the π- electron energy. The energy $E(G)$ of a graph G is defined to be the sum of the absolute values of its eigenvalues. Hence if $A(G)$ is the adjacency matrix of G and if $\lambda_1,\ \lambda_2,\ \cdots,\ \lambda_n$ are its eigenvalues, then $E(G) = \sum_{i=1}^{n} |\lambda_i|$. Numerous review articles have been written on the energy of graphs, see e.g. [1]-[10].

One of the ways of studying graphs is to make use of matrices. Several graph matrices have been defined and used in literature. Apart from the adjacency matrix, the incidency and Laplacian matrices are the most important ones. Another matrix, the maximum degree matrix was defined by Adiga and Smitha in [11]. Let G be a simple graph with n vertices $v_1,\ v_2,\ \cdots,\ v_n$ and let d_i be the degree of v_i for $i = 1,\ 2,\ \cdots,\ n$. Define

$$d_{ij} = \begin{cases} \max\{d_i, d_j\} & if\ v_i\ and\ v_j\ are\ adjacent \\ 0 & otherwise \end{cases}$$

Then the $n\times n$ matrix $M(G) = (d_{ij})$ is called the maximum degree matrix of G, [11]. Let $\mu_1,\ \mu_2,\ \cdots,\ \mu_n$ be the maximum degree eigenvalues of $M(G)$. Since $M(G)$ is a real symmetric matrix with zero trace, these maximum degree eigenvalues are real with sum equal to zero. That is,

$$\sum_{i=1}^{n} \mu_i \ = \ 0.$$

The maximum degree energy of a graph G is defined as

$$E_M(G) = \sum_{i=1}^{n} |\mu_i| \,.$$

It is shown that if the maximum degree energy of a graph is rational, then it must be an even integer, [11].

In this paper, we establish bounds for maximum degree eigenvalues of graphs, in particular, for unicyclic graphs. We find sharp bounds for the maximum degree eigenvalues of some classes of graphs and also find different bounds for maximum degree energy of these graph classes. In the final section of the paper, we calculate the maximum degree energy of some certain graphs where one edge of them is deleted. By applying the same operation successively, the maximum degree energy of large graphs can be calculated by reducing the number of edges one by one.

The following result about the sum of squares of the maximum degree eigenvalues is one of the main tools for our calculations:

Theorem 1.1. [11] *If $\mu_1,\ \mu_2,\ \cdots,\ \mu_n$ are the maximum degree eigenvalues of a graph G, then*

$$\sum_{i=1}^{n} \mu_i^2 = 2\sum_{i=1}^{n}(a_i + b_i)d_i^2$$

where a_i denotes the number of vertices in the neighborhood of v_i whose degrees are less than d_i and b_i denotes the number of vertices v_j with $j > i$, in the neighborhood of v_i whose degrees are equal to d_i.

It is important to note that this sum is independent from the choice of the labeling of the vertices. We also note the following inequality:

Theorem 1.2. [11] *If G is a graph of order n, then*

$$\sqrt{2\sum_{i=1}^{n}(a_i + b_i)d_i^2 + n(n-1)P^{2/n}} \leq E_M G \leq \sqrt{2n\sum_{i=1}^{n}(a_i + b_i)d_i^2}$$

where $P = \prod_{i=1}^{n} |\mu_i|$.

The following useful upper bound was obtained for the maximum degree eigenvalues of a graph:

Theorem 1.3. [11] *If G is graph of order n, then for any maximum degree eigenvalue μ_j, we have $|\mu_j| \leq (n-1)^2$.*

If a graph is the disjoint union of two smaller graphs, then its spectrum can be stated in terms of smaller spectrums as follows:

Lemma 1.4. *Let G_1 and G_2 be two disjoint graphs and let G be their union. The spectrum of $M(G)$ is the union of the spectra of $M(G_1)$ and $M(G_2)$ with multiplicities added up.*

Proof. We can easily observe that maximum degree matrix of G has the diagonal block shape

$$M(G) = \begin{pmatrix} M(G_1) & O \\ O & M(G_2) \end{pmatrix}$$

with respect to a suitable vertex re-ordering. Thus the spectrum of $M(G)$ is obtained as the union of the spectra of $M(G_1)$ and $M(G_2)$ as stated. □

This result can easily be generalized to a finite number of graphs:

Theorem 1.5. *Let $G_1, \ G_2, \ \cdots, \ G_n$ be the connected components of G, then maximum degree energy of G is given bu*

$$E_M(G) \ = \ E_M(G_1) + E_M(G_2) + \cdots + E_M(G_n).$$

Proof. This follows from Lemma 1.4 and the definition of maximum degree energy. □

2. Bounds for maximum degree eigenvalues

We have the below upper bound for maximum degree eigenvalues:

Theorem 2.1. *If G is a graph of order n, then for any maximum degree eigenvalue μ_j, we have*

$$|\mu_j| \leq \sqrt{\frac{2(n-1)}{n}\sum_{i=1}^{n}(a_i+b_i)d_i^2} \tag{1}$$

where $a_i, \ b_i$ are the same with Theorem 1.1.

Proof. We have

$$\begin{aligned} \textstyle\sum_{i=1}^{n} \mu_i &= 0 \\ \textstyle\sum_{i=1}^{n} \mu_i^2 &= 2\textstyle\sum_{i=1}^{n}(a_i+b_i)d_i^2. \end{aligned}$$

Substituting $x_i = 1$ and $y_i = \mu_i, \ i = 1, 2, \cdots, j-1, j+1, \cdots, n$ in the Cauchy-Schwartz inequality, we get

$$\left(\sum_{i=1, i\neq j}^{n} \mu_i\right)^2 \leq (n-1) \sum_{i=1, i\neq j} \mu_i^2. \tag{2}$$

Substituting Eqn. (1) in Eqn. (2), we get

$$\begin{aligned} \mu_j^2 &\leq (n-1)\left(2\textstyle\sum_{i=1}^{n}(a_i+b_i)d_i^2 - \mu_j^2\right), \\ n\mu_j^2 &\leq 2(n-1)\textstyle\sum_{i=1}^{n}(a_i+b_i)d_i^2. \end{aligned}$$

Therefore the required result is obtained. □

2.1. **Bounds for some classes of graphs.** Some graph classes are more frequently used than others. Here we obtain bounds on maximum degree eigenvalues for some of such graph classes:

Corollary 2.2. *If G is a path graph P_n, then*

$$|\mu_j| \leq \sqrt{\frac{8}{n}(n-1)}.$$

Proof. If G is a path graph P_n, then $\sum_{i=1}^{n}(a_i + b_i)d_i^2 = 4(n-1)$. Hence we obtain the result. □

Corollary 2.3. *If G is a cycle graph C_n with $n \geq 3$, then*

$$|\mu_j| \leq \sqrt{8(n-1)}.$$

Proof. As $\sum_{i=1}^{n}(a_i + b_i)d_i^2 = 4n$, the result follows. □

Corollary 2.4. *If G is a complete graph K_n, then*

$$|\mu_j| \leq (n-1)^2.$$

Proof. If G is a complete graph K_n, then $\sum_{i=1}^{n}(a_i + b_i)d_i^2 = \frac{n(n-1)^3}{2}$. Hence the result follows. □

Corollary 2.5. *If G is a complete bipartite graph $K_{m,n}$ with $m \geq n$, then*

$$|\mu_j| \leq \sqrt{\frac{8mn^3(m+n-1)}{m+n}}.$$

Proof. If G is a complete bipartite graph $K_{m,n}$ with $m \geq n$, then it can be easily calculated that $\sum_{i=1}^{n}(a_i + b_i)d_i^2 = 4mn^3$. Hence we obtain the result. □

The following special case can be obtained by substituting $m = n-1$ and $n = 1$:

Corollary 2.6. *If G is a star graph S_n, then*

$$|\mu_j| \leq 2(n-1)\sqrt{\frac{2}{n}}.$$

Corollary 2.7. *If G is a crown graph on $2n$ vertices, then*

$$|\mu_j| \leq (n-1)\sqrt{(2n-1)(n-1)}.$$

Proof. If G is a crown graph on $2n$ vertices, then $\sum_{i=1}^{n}(a_i+b_i)d_i^2 = n(n-1)^3$. This gives the required result. □

2.2. **Unicyclic graphs.** We shall introduce some new graph classes to establish our results on unicyclic graphs. Let $G(n, l, k)$ denote the set of all unicyclic graphs on n vertices with girth l having k pendant vertices. Let S_n^l be the graph obtained by identifying the center of S_{n-l+1} with any vertex of C_l. Let P_n^l be the graph obtained by identifying one pendant vertex of the path P_{n-l+1} with any vertex of C_l. By $R_n^{l,k}$, we denote the graph obtained by identifying one pendant vertex of the path $P_{n-l-k+1}$ with one pendant vertex of S_{l+k}^l. We denote by $Q_n^{l,k}$ the graph obtained by attaching k pendant edges to the pendant vertex of P_{n-k}^l. Let $U_{n,l}$ be the unicyclic graph obtained from the cycle $C_l = v_1 v_2 \cdots v_l v_1$ by attaching $n - 2l + 1$ pendant vertices to v_1 and a pendant vertex to each of other vertices on C_l. That is $U_{n,l}$ has $n - l$ pendant vertices. If $n = 2l$, then one pendant vertex will be attached to each vertex of C_l. Also it is clear that $S_n^n = P_n^n = C_n$. The following figures illustrate S_n^l, P_n^l, $R_n^{l,k}$, $Q_n^{l,k}$ and $U_{n,l}$.

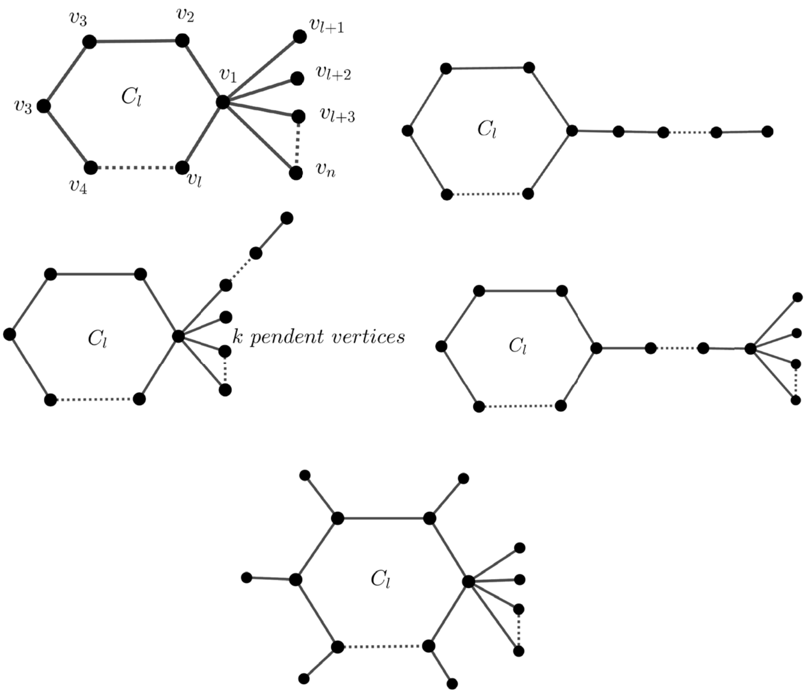

FIGURE 1. The unicyclic graphs S_n^l, P_n^l, $R_n^{l,k}$, $Q_n^{l,k}$ and $U_{n,l}$, respectively.

Corollary 2.8. *For the unicyclic graph S_n^l, we have*

$$|\mu_j| \leq \sqrt{\frac{2(n-1)}{n}\left((n-l+2)^3 + 4(l-2)\right)}.$$

Proof. For S_n^l, recall that we have

$$\sum_{i=1}^{n}(a_i + b_i)d_i^2 = (n-l+2)^3 + 4(l-2). \tag{3}$$

Hence we obtain the required result. □

Corollary 2.9. *For the unicyclic graph P_n^l, we have*

$$|\mu_j| \leq \sqrt{8(n-1) + \frac{18(n-1)}{n}}.$$

Proof. For the unicyclic graph P_n^l, we have $\sum_{i=1}^{n}(a_i+b_i)d_i^2 = 4(n-4)+25 = 4n+9$. Hence the result is obtained. □

Corollary 2.10. *For the unicyclic graph $U_{n,l}$, we have*

$$|\mu_i| \leq \sqrt{\frac{2(n-1)}{n}\left((n-2l+3)^3+18l-27\right)}.$$

Proof. For the unicyclic graph $U_{n,l}$, we have $\sum_{i=1}^{n}(a_i+b_i)d_i^2 = (n-2l+3)^3+2(l-2)\cdot 3^2+3^2 = (n-2l+3)^3+18l-27$. Hence the result follows. □

If $n=2l$, then each vertex on the cycle will be connected to one pendant vertex and hence $\sum_{i=1}^{n}(a_i+b_i)d_i^2 = 9n$. Hence $|\mu_i| \leq \sqrt{18(n-1)}$ is obtained as required.

Corollary 2.11. *For the unicyclic graph $R_n^{l,k}$, we have*

$$|\mu_j| \leq \sqrt{\frac{2(n-1)}{n}\left((k+2)^3+4(n-k-2)\right)}.$$

Proof. For $R_n^{l,k}$, we have

$$\sum_{i=1}^{n}(a_i+b_i)d_i^2 = (k+2)^3+4(n-k-2). \tag{4}$$

Hence the result follows. □

Corollary 2.12. *For the unicyclic graph $Q_n^{l,k}$, we have*

$$|\mu_j| \leq \sqrt{\frac{2(n-1)}{n}\left((k+1)^3+4(n-k)+7\right)}.$$

Proof. For $Q_n^{l,k}$, we have $\sum_{i=1}^{n}(a_i+b_i)d_i^2 = (k+1)^3+4(n-k)+7$ implying the result. □

As one may notice, the sum $\sum_{i=1}^{n}(a_i+b_i)d_i^2$ appears in many calculations. Therefore we shall now introduce the notion of vertex contribution as follows:

Definition 2.13. *Let v_i be a vertex of a graph G with degree d_i. We call the number $(a_i+b_i)d_i^2$ as the contribution of the vertex v_i.*

In most graphs, especially in unicyclic graphs, there are pendant vertices. Therefore, to know that their contribution is zero will be a very practical information:

Lemma 2.14. *If v_i is a pendant vertex of a connected graph G, then the contribution of v_i is zero.*

Proof. Let v_i be a pendant vertex of degree d_i and u_i be its unique neighbour. $d(u_i) \geq 2$ as G is connected. Hence $a_i = 0$ as there are no neighbours of v_i having degree less than $d(v_i) = 1$ and $b_i = 0$ as there are no neighbours of v_i with degree equal to $d(v_i) = 1$. Hence the contribution is zero. □

Theorem 2.15. *If $n = k + l$, then*

$$\sum_{i=1}^{n}\mu_i^2(S_n^l) = \sum_{i=1}^{n}\mu_i^2(R_n^{l',k})$$

for every l' such that $2 \leq l' \leq l$.

Proof. Recall that the labeling of the vertices doesn't effect the sum $\sum_{i=1}^{n}(a_i+b_i)d_i^2$. Hence we label S_n^l as in Fig. 1. First note that $S_n^l = R_n^{l,k}$, so the result is true for $l^{'} = l$. For the remaining cases, let $1 \le t \le l-2$ and $l^{'} = l-t$. The graph $R_n^{l-t,k}$ is obtained by carrying t vertices of degree 2 on the cycle on to the branch of G having vertices v_1 and v_{l+1} (other branches can also be chosen alternatively). Let $R_n^{l-t,k}$ be labeled as below: We form

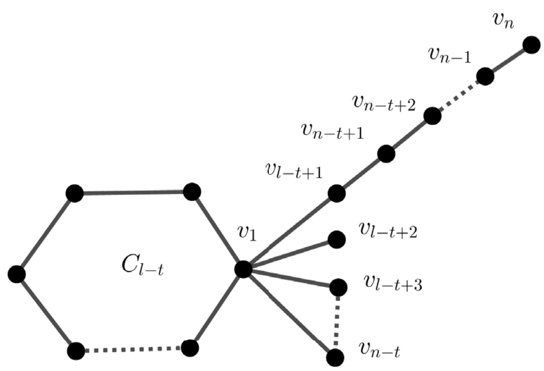

FIGURE 2. $R_n^{l-t,k}$

the following two tables for the graphs S_n^l and $R_n^{l-t,k}$.

So $\sum_{i=1}^{n}\mu_i^2(S_n^l) = (n-l+2)^3+4(l-2)$ and $\sum_{i=1}^{n}\mu_i^2(R_n^{l-t,k}) = (k+2)^3+4(l-2)$ and these are equal by the assumption. So the result follows. □

Theorem 2.16. *Let $n \ge 4$. The spectrum of the unicyclic graph S_n^3 consists of 0 with multiplicity $n-4$, -2 with multiplicity 1 and the three roots of the cubic polynomial $x^3-2x^2-(n-1)^3x+2(n-3)(n-1)^2 = 0$.*

Proof. The maximum degree matrix of S_n^3 according to the vertex labeling shown in Fig. 1 is of order $n \times n$ and is given by

$$M(S_n^3) = \begin{pmatrix} A_{3\times 3} & B_{3\times(n-3)} \\ B^T_{(n-3)\times 3} & O_{(n-3)\times(n-3)} \end{pmatrix}$$

where $A = \begin{pmatrix} 0 & n-1 & n-1 \\ n-1 & 0 & 2 \\ n-1 & 2 & 0 \end{pmatrix}$, $B = \begin{pmatrix} n-1 & n-1 & \cdots & n-1 \\ 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$ and O is the null matrix of size $(n-3)\times(n-3)$.

If R_i is the i^{th} row of the determinant $|\mu I - M(S_n^3)|$, then $R_2 = (n-1, -\mu, 2, 0, \cdots, 0)$ and $R_3 = (n-1, 2, -\mu, 0, \cdots, 0)$. Replacing R_2 by $R_2 - R_3$, we get the second row as $(\mu+2)(0, -1, 1, 0, \cdots, 0)$. Hence one of the maximum degree eigenvalues of $M(S_n^3)$ is found to be -2.

Replacing R_i by $R_i - R_{i+1}$ for $i = 4, 5, \cdots, n-1$, we conclude that μ is the common factor at each row between 4th and $(n-1)$-th. Hence

Table 1. For S_n^l

i	d_i	a_i	b_i	$(a_i+b_i)d_i^2$
1	$n-l+2$	$n-l+2$	0	$(n-l+2)^3$
2	2	0	1	4
3	2	0	1	4
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$l-1$	2	0	1	4
l	2	0	0	0
$l+1$	1	0	0	0
$l+2$	1	0	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	1	0	0	0

Table 2. For $R_n^{l-t,k}$

i	d_i	a_i	b_i	$(a_i+b_i)d_i^2$
1	$l+2$	$k+2$	0	$(k+2)^3$
2	2	0	1	4
3	2	0	1	4
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$l-t-1$	2	0	1	4
$l-t$	2	0	0	0
$l-t+1$	2	0	1	4
$l-t+2$	1	0	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$n-t$	1	0	0	0
$n-t+1$	2	0	1	4
$n-t+2$	2	0	1	4
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$n-1$	2	1	0	4
n	1	0	0	0

0 is a maximum degree eigenvalue of $M(S_n^3)$ with multiplicity $n-4$. Using elementary mathematical simplifications we get the cubic polynomial. Therefore the required result is obtained. □

Theorem 2.17. *Let $n \geq 5$. Then the maximum degree energy of the unicyclic graph S_n^4 having $k = n-4$ pendant vertices is*

$$E_M(S_n^4) = \sqrt{2}\left[\sqrt{n\,(t+4)+\sqrt{Y}} + \sqrt{n\,(t+4)-\sqrt{y}}\right]$$

where $t = k(k+2)$ and $y = n^2(t+4)^2 - 32t^2$.

Proof. The maximum degree matrix of S_n^4 according to the vertex labeling shown in Fig. 1 is of size $n \times n$ and given by

$$M(S_n^4) = \begin{pmatrix} A_{4\times 4} & B_{4\times(n-4)} \\ B^T_{(n-4)\times 4} & O_{(n-4)\times(n-4)} \end{pmatrix}$$

where $A = \begin{pmatrix} 0 & n-2 & 0 & n-2 \\ n-2 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 \\ n-2 & 0 & 2 & 0 \end{pmatrix}$, $B = \begin{pmatrix} n-2 & n-2 & \cdots & n-2 \\ 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$ and O is the null matrix of size $(n-4)\times(n-4)$. The maximum degree characteristic equation of $M(S_n^4)$ is

$$\mu^{n-4}(\mu^4 - n\left((n-2)(n-4)+4\right)\mu^2 + 8(n-4)(n-2)^2) = 0.$$

Hence maximum degree eigenvalues are 0 with multiplicity $n-4$, $\sqrt{\frac{n(t+4)+\sqrt{y}}{2}}$, $-\sqrt{\frac{n(t+4)+\sqrt{y}}{2}}$, $\sqrt{\frac{n(t+4)-\sqrt{y}}{2}}$ and $-\sqrt{\frac{n(t+4)+\sqrt{y}}{2}}$. Therefore the required maximum degree energy will be

$$E_M(S_n^4) = \sqrt{2}\left[\sqrt{n\,(t+4)+\sqrt{y}} + \sqrt{n\,(t+4)-\sqrt{y}}\right].$$

□

3. Bounds for maximum degree energy

In this section we establish different lower bounds for maximum degree energy $E_M(G)$.

Theorem 3.1. *If G is a simple graph with n vertices, then*

$$2\sqrt{M} \le E_M(G) \le \sqrt{2nM}$$

where $M = \sum_{i=1}^n (a_i+b_i)d_i^2$ denotes the total vertex contribution and a_i, b_i are the same with Theorem 1.1.

Proof. We have

$$0 = \left(\sum_{i=1}^{i=n} \mu_i\right)^2 = \sum_{i=1}^{i=n} \mu_i^2 + 2\sum_{1\le i\le j\le n} \mu_i\mu_j.$$

By Theorem 1.1, we get

$$\sum_{1\le i\le j\le n} \mu_i\mu_j = -\sum_{i=1}^{n}(a_i+b_i)d_i^2.$$

We have

$$\begin{aligned} E_M(G)^2 &= \left(\sum_{i=1}^n |\mu_i|\right)^2 \\ &= \sum_{i=1}^{i=n} \mu_i^2 + 2\sum_{1\le i\le j\le n} |\mu_i\mu_j| \\ &\ge \sum_{i=1}^{i=n} \mu_i^2 + 2\left|\sum_{1\le i\le j\le n} \mu_i\mu_j\right| \\ &= 4\sum_{i=1}^{n}(a_i+b_i)d_i^2 = 4M. \end{aligned}$$

Therefore,

$$E_M(G) \geq 2\sqrt{M}.$$

Combining this with inequality in Theorem 1.2, we get

$$2\sqrt{M} \leq E_M(G) \leq \sqrt{2nM}.$$

□

Using Theorem 3.1 and Corollaries 2.8-2.12, we have the following for $n > l \geq 3$

(5) $$2\sqrt{(n-l+2)^3 + 4(l-2)} \leq E_M(S_n^l) \leq \sqrt{2n\left((n-l+2)^3 + 4(l-2)\right)},$$

(6) $$2\sqrt{4n+9} \leq E_M(P_n^l) \leq \sqrt{2n\,(4n+9)},$$

(7) $$2\sqrt{(n-2l+3)^3 + 18l - 27} \leq E_M(U_{n,l}) \leq \sqrt{2n\left((n-2l+3)^3 + 18l - 27\right)},$$

(8) $$2\sqrt{(k+2)^3 + 4(n-k-2)} \leq E_M(R_n^{l,k}) \leq \sqrt{2n\left((k+2)^3 + 4(n-k-2)\right)},$$

(9) $$2\sqrt{(k+1)^3 + 4(n-k) + 7} \leq E_M(Q_n^{l,k}) \leq \sqrt{2n\left((k+1)^3 + 4(n-k) + 7\right)}.$$

Recall that we have obtained the eigenvalues of $M(S_n^3)$ as 0 with multiplicity $n-4$, -2 with multiplicity 1 and the three roots α_1, α_2 and α_3 of the cubic polynomial $x^3 - 2x^2 - (n-1)^3x + 2(n-3)(n-1)^2 = 0$. As

(10) $$\alpha_1 + \alpha_2 + \alpha_3 = 2,$$

we have

$$2 = |\alpha_1 + \alpha_2 + \alpha_3| \leq |\alpha_1| + |\alpha_2| + |\alpha_3|$$

implying that $|\alpha_1| + |\alpha_2| + |\alpha_3| \geq 2$. Hence

$$\begin{aligned} E_M(S_n^3) &= |\alpha_1| + |\alpha_2| + |\alpha_3| + |-2| + 0 + 0 + \cdots + 0 \\ &= |\alpha_1| + |\alpha_2| + |\alpha_3| + 2 \\ &\geq 4. \end{aligned}$$

By substituting $l = 3$ in the left hand side inequality in Eqn. (5) above, we can improve the lower bound for the maximum degree energy of S_n^3 as below:

Corollary 3.2. *Maximum degree energy of S_n^3 satisfies the following inequality:*

$$E_M(S_n^3) \geq 2\sqrt{(n-1)^3 + 4}.$$

Note that

(11) $$\alpha_1\alpha_2 + \alpha_2\alpha_3 + \alpha_3\alpha_1 = -(n-1)^3$$

and

(12) $$\alpha_1\alpha_2\alpha_3 = -2(n-3)(n-1)^2.$$

By Eqn. (12), the cubic equation has one negative root or all three are negative. By Eqn. (10), it is clear that all three roots cannot be negative. Hence the cubic surely has one negative root. The other two must be positive. Let us say that α_1 and α_2 are positive and α_3 is negative. Therefore, although we do not know the exact values of the three maximum degree eigenvalues

$\alpha_1,\ \alpha_2$ and α_3 of the above cubic polynomial explicitly, we can determine the maximum degree energy of S_n^3:

Theorem 3.3. *Maximum degree energy of* S_n^3 *is*

$$E_M(S_n^3) = 4 - 2\alpha_3$$

where α_3 *is the unique negative root of the cubic polynomial* $x^3 - 2x^2 - (n-1)^3x + 2(n-3)(n-1)^2 = 0$.

Lemma 3.4. *Let* $\mu_1,\ \mu_2,\ \cdots,\ \mu_n$ *be the maximum degree eigenvalues of* G *where* μ_1 *is the greatest one. Then*

$$\sqrt{\frac{2M}{n}} \leq \mu_1 \leq \sqrt{2M} \tag{13}$$

where M *is the same with Theorem 3.1.*

Proof. We have

$$\mu_1^2 + \mu_2^2 + \cdots + \mu_n^2 = 2\sum_{i=1}^{n}(a_i + b_i)d_i^2 \tag{14}$$

$$\mu_1^2 \leq 2\sum_{i=1}^{n}(a_i + b_i)d_i^2$$

That is

$$\mu_1 \leq \sqrt{2\sum_{i=1}^{n}(a_i + b_i)d_i^2} = \sqrt{2M}$$

showing the second inequality. Again from (14), we have

$$n\mu_1^2 \geq 2\sum_{i=1}^{n}(a_i + b_i)d_i^2$$

$$\mu_1 \geq \sqrt{\frac{2M}{n}}.$$

Therefore, we have the desired result. □

Theorem 3.5. *If* G *is a simple graph with* n *vertices, then*

$$E_M(G) \leq \frac{2M + \sqrt{2M(n-1)(n^2 - 2M)}}{n}$$

where M *is the same with Theorem 3.1.*

Proof. Let $\mu_1,\ \mu_2,\ \cdots,\ \mu_n$ be the eigenvalues of G where μ_1 is the greatest eigenvalue. By the Cauchy-Schwartz inequality

$$\left(\sum_{i=2}^{n}|\mu_i|\right)^2 \leq (n-1)\sum_{i=2}^{n}|\mu_i|^2 \quad = (n-1)\left(2\sum_{i=1}^{n}(a_i + b_i)d_i^2 - \mu_1^2\right).$$

Now

$$\begin{aligned} E_M(G) &= \mu_1 + \sum_{i=2}^{n}|\mu_i| \\ &\leq \mu_1 + \sqrt{(n-1)\left(2\sum_{i=1}^{n}(a_i + b_i)d_i^2 - \mu_1^2\right)}. \\ &= \mu_1 + \sqrt{(n-1)\left(2M - \mu_1^2\right)}. \end{aligned}$$

Now consider the derivative of the expression on the right hand side with respect to μ_1 to obtain

$$\frac{d}{d\mu_1}\left(\mu_1+\sqrt{(n-1)\left(2M-\mu_1^2\right)}\right)=1-\frac{\mu_1\sqrt{n-1}}{\sqrt{2M-\mu_1^2}}$$

which is positive for $0<\mu_1<\sqrt{2M/n}$ and negative for $\sqrt{2M/n}<\mu_1<\sqrt{2M}$. Since by Lemma 3.4, the upper bound of $E_M(G)$ is decreasing implying

$$\begin{aligned} E_M(G) &\leq \mu_1+\sqrt{(n-1)\left(2\sum_{i=1}^{n}(a_i+b_i)d_i^2-\mu_1^2\right)} \\ &\leq \tfrac{2M}{n}+\sqrt{(n-1)\left(2M-\left(\tfrac{2M}{n}\right)^2\right)}. \end{aligned}$$

Hence the result is obtained. □

There is the following nice relation between the number of vertices and the sum of squares of the maximum degree eigenvalues:

Corollary 3.6. *If $2M\leq n$ then $E_M\leq n$.*

Proof. By Theorem 1.2, we have

$$E_MG\leq\sqrt{2Mn}\leq n.$$

□

Corollary 3.7. *If $M\leq\frac{n^2+n^{3/2}}{4}$, then $E_M(G)\leq\frac{n}{2}(1+\sqrt{n})$.*

Proof. Consider the bound in Theorem 3.5 as a function of M:

$$g(M)=\frac{2M}{n}+\sqrt{(n-1)\left(2M-\left(\frac{2M}{n}\right)^2\right)}.$$

Differentiating with respect to M gives

$$g^{'}(M)=\frac{2}{n}-\frac{\sqrt{n-1}(4M-n^2)}{n\sqrt{2M(n^2-2M)}}.$$

Hence $g^{'}(M)$ is positive for $M<\frac{n^2+n^{3/2}}{4}$ and negative for $M>\frac{n^2+n^{3/2}}{4}$. Thus we have

$$E_MG\leq g(M)\leq g\left(\frac{n^2+n^{3/2}}{4}\right)=\frac{n}{2}(1+\sqrt{n}).$$

□

Theorem 3.8. *If G is a simple graph, then*

$$E_M(G)\geq\sqrt{2nM-\frac{(n(P-p))^2}{4}} \tag{15}$$

where M is the same with Theorem 3.1, $p=\min\{|\mu_i|\}$, $P=\max\{|\mu_i|\}$ for $i=1,\ 2,\ \cdots,\ n$.

Proof. If a_i, b_i are non-negative real numbers, then $\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \frac{n^2}{4}(M_1M_2 - m_1m_2)^2$ where $M_1 = max\{a_i\}$, $M_2 = max\{b_i\}$, $m_1 = min\{a_i\}$, $m_2 = min\{b_i\}$ for $i = 1,\ 2,\ \cdots,\ n$, [12].

Take $a_i = 1$, $b_i = |\mu_i|$. Then $M_1 = m_1 = 1$. Let $m_2 = \min\{|\mu_i|\} = p$ and $M_2 = \max\{|\mu_i|\} = P$. Then the inequality becomes

$$n\sum_{i=1}^{n} |\mu_i|^2 - \left(\sum_{i=1}^{n} |\mu_i|\right)^2 \leq \frac{n^2}{4}(P-p)^2$$

and hence

$$2n\sum_{i=1}^{n}(a_i + b_i)d_i^2 - E_M(G)^2 \leq \frac{n^2}{4}(P-p)^2.$$

Therefore

$$E_M(G) \geq \sqrt{2n\sum_{i=1}^{n}(a_i + b_i)d_i^2 - \frac{n^2}{4}(P-p)^2}.$$

□

Theorem 3.9. *Let G be simple graph with n vertices and m edges. Then*

$$E_M(G) \geq \sqrt{2nM - \alpha(n)(P-p)^2} \tag{16}$$

where M, p, P are the same with Theorem 3.8 and $\alpha(n) = n\lfloor n/2 \rfloor \left(1 - \frac{1}{n}\lfloor n/2 \rfloor\right)$.

Proof. If a_i, b_i are non-negative real numbers, then $|n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i| \leq \alpha(n)(A-a)(B-b)$ where a, b, A and B are real constants such that $a \leq a_i \leq A$, $b \leq b_i \leq B$ for $1 \leq i \leq n$. Further $\alpha(n) = n\lfloor n/2 \rfloor \left(1 - \frac{1}{n}\lfloor n/2 \rfloor\right)$, [13]. Then by substituting $a_i = b_i = |\mu_i|$, $a = b = \min\{|\mu_i|\} = p$ and $A = B = \max\{|\mu_i|\} = P$, we get

$$\left|n\sum_{i=1}^{n} |\mu_i|^2 - (E_M(G))^2\right| \leq \alpha(n)(P-p)^2.$$

Hence

$$\left|2n\left(\sum_{i=1}^{n}(a_i + b_i)d_i^2\right) - (E_M(G))^2\right| \leq \alpha(n)(P-p)^2.$$

Therefore the result follows. □

Remark 3.10. *Since $\alpha(n) \leq \frac{n^2}{4}$ by Eqns. (15) and (16), we can easily observe that the inequality in Eqn. (16) is sharper than the inequality in Eqn. (15).*

Theorem 3.11. *Let G be a simple graph with n vertices and m edges. Then*

$$E_M(G) \geq \frac{2M + npP}{P + p}$$

where M, p, P are the same with Theorem 3.8.

Proof. If a_i, b_i are non-negative real numbers, then $\sum_{i=1}^{n} b_i^2 + p \cdot P\sum_{i=1}^{n} a_i^2 \leq (p+P)\left(\sum_{i=1}^{n} a_i b_i\right)$ where p and P are real constants such that $pa_i \leq b_i \leq Pa_i$

for each i so that $1 \leq i \leq n$, [12]. Then by substituting $a_i = 1$, $b_i = |\mu_i|$, $p = \min\{|\mu_i|\}$ and $P = \max\{|\mu_i|\}$, we get

$$\sum_{i=1}^{n} |\mu_i|^2 + npP \leq (p+P) \sum_{i=1}^{n} |\mu_i|$$

and hence

$$2\sum_{i=1}^{n}(a_i+b_i)d_i^2 + npP \leq (p+P)E_M(G).$$

$$2M + npP \leq (p+P)E_M(G).$$

Therefore,

$$E_M(G) \geq \frac{2M+npP}{P+p}.$$

□

Theorem 3.12. *If G is a simple graph with n vertices and m edges, then*

$$E_M(G) \geq \frac{2\sqrt{2npPM}}{p+P},$$

where M, p, P are the same with Theorem 3.8.

Proof. If a_i, b_i are non-negative real numbers, then

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} a_ib_i\right)^2$$

where $M_1 = max\{a_i\}$, $M_2 = max\{b_i\}$, $m_1 = min\{a_i\}$, $m_2 = max\{b_i\}$ for $i = 1, 2, \cdots, n$, see [14].

Take $a_i = 1$, $b_i = |\mu_i|$, then $M_1 = m_1 = 1$. Let $m_2 = \min\{|\mu_i|\} = p$ and $M_2 = \max\{|\mu_i|\} = P$, then the inequality becomes

$$n\left(\sum_{i=1}^{n} |\mu_i|^2\right) \leq \frac{1}{4}\frac{(p+P)^2}{pP}\left(E_M(G)\right)^2.$$

Hence

$$n\left(2\sum_{i=1}^{n}(a_i+b_i)d_i^2\right) \leq \frac{1}{4}\frac{(p+P)^2}{pP}\left(E_M(G)\right)^2.$$

Therefore

$$E_M(G) \geq \frac{2\sqrt{2npPM}}{p+P}.$$

□

4. Maximum degree energy for some classes of graphs

Theorem 4.1. *The maximum degree energy of a path graph of order n is*

$$E_M(P_n) \quad = 4\sum_{k=1}^{n}\left|\cos\left(\frac{k\pi}{n+1}\right)\right|.$$

Proof. The maximum degree matrix of a path graph P_n is a tridiagonal matrix and is of the form

$$\begin{bmatrix} c & a & & & \\ b & c & a & & \\ & b & c & & \\ & & & c & a \\ & & & b & c \end{bmatrix}$$

where $a = b = 2$ and $c = 0$. Hence the eigenvalues are $4\cos\left(\frac{k\pi}{n+1}\right)$, $k = 1, 2, \cdots n$, [15]. Therefore,

$$E_M(P_n) \quad = 4\sum_{k=1}^{n}\left|\cos\left(\frac{k\pi}{n+1}\right)\right|.$$

□

Theorem 4.2. *The maximum degree energy of a cycle graph of order n, ($n \geq 3$) is given by*

$$E_M(C_n) \quad = 4\sum_{k=0}^{n-1}\left|\cos\left(\frac{2k\pi}{n}\right)\right|,\ n \geq 3.$$

Proof. The maximum degree matrix of a cycle graph C_n for $n \geq 3$ is a circulant matrix of size $n \times n$ and is of the form

$$\begin{bmatrix} 0 & 2 & 0 & \cdots & 0 & 2 \\ 2 & 0 & 2 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 2 & 0 & 0 & \cdots & 2 & 0 \end{bmatrix}$$

The eigenvalues of the circulant matrix are $\mu_k = 0 + 2\cdot\omega_k + 0\cdot(\omega_k)^2 + \cdots + 2\cdot(\omega_k)^{n-1}$ where $\omega_k = e^{\left(\frac{2\pi k}{n}\right)\cdot i}$, $k = 0,\ 1,\ 2,\ \cdots,\ n-1$. Hence

$$\begin{aligned}\mu_k &= 2\left[\omega_k + \omega_k^{n-1}\right] \\ &= 2\cdot\left[\cos\left(\frac{2\pi k}{n}\right) + i\sin\left(\frac{2\pi k}{n}\right) + \cos\left(\frac{2\pi k(n-1)}{n}\right) + i\sin\left(\frac{2\pi k(n-1)}{n}\right)\right] \\ &= 4\cos\left(\frac{2k\pi}{n}\right),\ k = 0,\ 1,\ 2,\ \cdots,\ n-1.\end{aligned}$$

Therefore

$$E_M(C_n) = 4\sum_{k=0}^{n-1}\left|\cos\left(\frac{2k\pi}{n}\right)\right|, n \geq 3.$$

□

Remark 4.3. *We can easily observe from Theorem 4.1 and Theorem 4.2 that*

$$E_M(P_n) \leq E_M(C_n).$$

Theorem 4.4. [11] *If G is a complete graph K_n, then $E_M(K_n) = 2(n-1)^2$.*

Theorem 4.5. *For $m \geq n$, the maximum degree energy of a complete bipartite graph is*

$$E_M(K_{m,n}) = 2\sqrt{nm^3}.$$

Proof. Let $m \geq n$. The maximum degree matrix of $K_{m,n}$ of order $m+n$ is

$$M(K_{m\cdot n}) = \begin{pmatrix} O_{m\times m} & A_{m\times n} \\ A^T_{m\times n} & O_{n\times n} \end{pmatrix}$$

where $A_{m\times n} = \begin{bmatrix} m & m & \cdots & m \\ m & m & \cdots & m \\ \cdot & \cdot & \cdots & \cdot \\ m & m & \cdots & m \end{bmatrix}$ and its spectrum would be

$$\begin{pmatrix} 0 & \sqrt{nm^3} & -\sqrt{nm^3} \\ m+n-2 & 1 & 1 \end{pmatrix}.$$

Therefore

$$E_M(K_{m,n}) = 2\sqrt{nm^3}.$$

□

Remark 4.6. *The maximum degree energy of a star graph is* $E_M(S_n) = 2\sqrt{(n-1)^3}$.

Theorem 4.7. *The maximum degree energy of a crown graph on* $2n$ *vertices is*

$$E_M(S_n^0) = 4(n-1)^2.$$

Proof. The maximum degree matrix of a crown graph on $2n$ with $n \geq 2$ vertices is

$$M(S_n^0) = \begin{pmatrix} O_{n\times n} & A_{n\times n} \\ A_{n\times n} & O_{n\times n} \end{pmatrix}$$

where

$$A_{n\times n} = \begin{bmatrix} 0 & n-1 & \cdots & n-1 \\ n-1 & 0 & \cdots & n-1 \\ \cdot & \cdot & \cdots & \cdot \\ n-1 & n-1 & \cdots & 0 \end{bmatrix}$$

and $O_{n\times n}$ is the null matrix of order n. The spectrum of $M(S_n^0)$ is

$$\begin{pmatrix} n-1 & -(n-1) & (n-1)^2 & -(n-1)^2 \\ n-1 & n-1 & 1 & 1 \end{pmatrix}.$$

Therefore

$$E_M(S_n^0) = 4(n-1)^2.$$

□

5. Maximum degree energy of graphs with one edge deleted

In graph theory, some operations play important role in finding and proving some required property or to give some extremal results. Some operations are needed to be applied only once while some others need to be applied successively. Amongst those operations, edge and vertex addition and deletion are frequently used ones. In this final section we obtain the maximum degree energy for certain graphs with one edge deleted. The same operation can be applied successively to obtain the maximum degree energy of a large graph by reducing the number of edges one by one. Our first case is the complete graph K_n:

Theorem 5.1. *Let e be an edge of the complete graph K_n. The maximum degree energy of $K_n - e$ is*

$$E_M(K_n - e) = (n-1)(n-3+\sqrt{n^2+2n-7}).$$

Proof. Let $v_1, v_2, \cdots, v_n$ be the vertex labeling of K_n and let $e = v_1 - v_2$. Then the maximum degree matrix of $M(K_n - e)$ is given by $M(K_n - e) = \begin{pmatrix} 0_{2\times 2} & (n-1)J_{2\times(n-2)} \\ (n-1)J_{(n-2)\times 2} & (n-1)(J-I)_{(n-2)} \end{pmatrix}$, where J is a matrix whose all entries are equal to 1 and its characteristic equation is

$$\lambda(\lambda^2 - (n-3)(n-1)\lambda - (n-1)^2(2n-4)) = 0.$$

Therefore the spectrum is found as

$$\begin{pmatrix} 1-n & \frac{(n-1)((n-3)+\sqrt{n^2+2n-7})}{2} & \frac{(n-1)((n-3)-\sqrt{n^2+2n-7})}{2} & 0 \\ n-3 & 1 & 1 & 1 \end{pmatrix}.$$

Therefore $E_M(K_n - e) = (n-1)(n-3+\sqrt{n^2+2n-7})$. □

Secondly, we illustrate the effect of edge deletion on maximum degree energy by using the special bipartite graph $K_{n,n}$:

Theorem 5.2. *Let e be an edge of a complete bipartite graph $K_{n,n}$. The maximum degree energy of $K_{n,n} - e$ is*

$$E_M(K_{n,n} - e) = 2n\sqrt{n^2+2n-3}.$$

Proof. Let $v_1, v_2, \cdots, v_n,\ u_1, u_2, \cdots, u_n$ be the vertex labeling of $K_{n,n}$ and let $e = v_n - u_n$.It is not difficult to form

$$M(K_{n,n} - e) = \begin{pmatrix} 0_{n\times n} & A \\ A & 0_{n\times n} \end{pmatrix}$$

where $A = \begin{pmatrix} (n-1)J_{(n-1)\times(n-1)} & (n-1)J_{(n-1)\times 1} \\ (n-1)J_{1\times(n-1)} & 0_{1\times 1} \end{pmatrix}$. Then the characteristic equation is

$$\lambda^{2n-4}(\lambda^2 + n(n-1)\lambda - n^2(n-1))(\lambda^2 - n(n-1)\lambda - n^2(n-1)) = 0.$$

Hence, the spectrum is

$$\begin{pmatrix} \frac{-n(n-1)+n\sqrt{n^2+2n-3}}{2} & \frac{-n(n-1)-n\sqrt{n^2+2n-3}}{2} & \frac{n(n-1)+n\sqrt{n^2+2n-3}}{2} & \frac{n(n-1)-n\sqrt{n^2+2n-3}}{2} & 0 \\ 1 & 1 & 1 & 1 & 2n-4 \end{pmatrix}.$$

Therefore $E_M(K_{n,n} - e) = 2n\sqrt{n^2+2n-3}$. □

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