Applicable Analysis and Discrete Mathematics
available online at http://pefmath.etf.rs

Appl. Anal. Discrete Math. **x** (xxxx), xxx–xxx.
https://doi.org/10.2298/AADM201227016A

UPPER BOUNDS ON THE ENERGY OF GRAPHS IN TERMS OF MATCHING NUMBER

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The energy of a graph G, $\mathcal{E}(G)$, is the sum of absolute values of the eigenvalues of its adjacency matrix. The matching number $\mu(G)$ is the number of edges in a maximum matching. In this paper, for a connected graph G of order n with largest vertex degree $\Delta \geq 6$ we present two new upper bounds for the energy of a graph: $\mathcal{E}(G) \leq (n-1)\sqrt{\Delta}$ and $\mathcal{E}(G) \leq 2\mu(G)\sqrt{\Delta}$. The latter one improves recently obtained bound

$$\mathcal{E}(G) \leq \begin{cases} 2\mu(G)\sqrt{2\Delta_e+1}, & \text{if } \Delta_e \text{ is even;} \\ \mu(G)(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}}), & \text{otherwise,} \end{cases}$$

where Δ_e stands for the largest edge degree and $a = 2(\Delta_e+1)$. We also present a short proof of this result and several open problems.

1. INTRODUCTION

For a graph G, denote the set of vertices and the set of edges of G by $V(G)$ and $E(G)$, respectively. The *adjacency matrix* of a graph G of order n, $A_G = [a_{ij}]$, is an $n \times n$ matrix, where $a_{ij} = 1$ if $v_iv_j \in E(G)$, and $a_{ij} = 0$, otherwise. The *energy* of a graph G, $\mathcal{E}(G)$, is defined as the energy of A_G. Note that since A_G is symmetric, $\mathcal{E}(G) = \sum_1^n |\lambda_i|$, where $\lambda_1 \geq \cdots \geq \lambda_n$ are eigenvalues of A_G. The concept of graph energy was first introduced by Gutman in 1978 [**8**]. The matching number $\mu(G)$ is the number of edges in a maximum matching of G. In this paper we present new upper bounds on graph energy in terms of its order and the largest vertex degree as well as in terms of matching number and the largest vertex degree.

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2020 Mathematics Subject Classification. 05C50, 05C70.
Keywords and Phrases. Energy (of graph), Graph energy, Matching number.

Both, energy and matching number have numerous applications in chemical graph theory, see [**10**]. Recently, a number of other bounds on graph energy, both upper and lower, has been communicated (see e.g., [**2, 3, 4, 7, 12, 16, 17, 20**], and the references cited therein), showing that this topic of research is timely and of current mathematical interest.

The paper is organized as follows. In Section 2 we present preliminary results needed for the remaining content of the paper. Section 3 includes three upper bounds on graph energy. For the first one, already known in the literature, in terms of matching number and the largest edge degree we present new, shorter proof. The remaining bounds are in terms of graph order (resp. matching number) and the largest vertex degree. In Section 4 we present two open problems.

2. PRELIMINARIES

Let $\varphi_G(x) = x^n + a_1x^{n-1} + \cdots + a_n$ be the characteristic polynomial of a graph G. We recall the Sachs theorem for the coefficients of the characteristic polynomial of a graph, that is

$$a_i = a_i(G) = \sum_{S \in \mathcal{L}_i} (-1)^{k(S)} 2^{c(S)},$$

where $\mathcal{L}_i$ denotes the set of Sachs graphs of G with i vertices, $k(S)$ is the number of components of S and $c(S)$ is the number of cycles contained in S. Then, $\mathcal{E}(G)$ can be expressed using the Coulson integral formula [**6, 13**]

$$\mathcal{E}(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[\left(\sum_{j=0}^{\lceil \frac{n}{2} \rceil} b_{2j} x^{2j} \right)^2 + \left(\sum_{j=0}^{\lceil \frac{n}{2} \rceil} b_{2j+1} x^{2j+1} \right)^2 \right] dx$$

where $b_i(G) = |a_i(G)|$, $i = 0, 1, \ldots, n$.

Assume that A is a symmetric real matrix whose rows and columns are indexed by $X = \{1, 2, \ldots, n\}$. Let $\{X_1, X_2, \ldots, X_m\}$ be a partition of X. Then A can be partitioned according to $\{X_1, X_2, \ldots, X_m\}$, that is,

$$A_G = \begin{bmatrix} A_{1,1} & \cdots & A_{1,m} \\ \vdots & \ddots & \vdots \\ A_{m,1} & \cdots & A_{m,m} \end{bmatrix},$$

where $A_{i,j}$ stands for the submatrix of A indexed by the rows of X_i and the columns of X_j. Denote the average row sum of $A_{i,j}$ by b_{ij}. Then the matrix $B = [b_{ij}]$ is called the quotient matrix of A. Furthermore, if the row sum of every block $A_{i,j}$ is constant, then the partition is called equitable.

Lemma 1. [**5**, Lemma 2.3.1] *Let A be a real, symmetric matrix. If A has an equitable partition and B is the corresponding quotient matrix, then each eigenvalue of B is also an eigenvalue of A.*

Next, we recall several results on graph energy and maximum matching that will be used in the sequel.

Theorem 2. [**1**] *Let G be a graph and $H_1, \ldots, H_k$ be some subgraphs of G. If $E(H_1), \ldots, E(H_k)$ is a partition of $E(G)$, then*

$$\mathcal{E}(G) \leq \sum_{i=1}^{k} \mathcal{E}(H_i).$$

Lemma 3. [**1**] *Let G be a graph and $H_1, \ldots, H_k$ be k vertex-disjoint induced subgraphs of G. Then $\mathcal{E}(G) \geq \sum_{i=1}^{k} \mathcal{E}(H_i)$.*

Theorem 4. [**13**, Theorem 4.19.] *Let H be an induced subgraph of a simple graph G. Then $\mathcal{E}(H) \leq \mathcal{E}(G)$, and equality holds if and only if $E(H) = E(G)$.*

A graph G of order n is called *hyperenergetic* if its energy is at least $2n - 2$. The following result implies that the energy of any graph G of order less than or equal to 7, is at most $2n - 2$.

Theorem 5. [**9**] *Hyperenergetic graphs on n vertices exist for all $n \geq 8$. There are no hyperenergetic graphs on less than 8 vertices.*

Theorem 6. (König's Theorem) [**14**, p.4] *Let $G = (V, E)$ be a bipartite graph. Then the size of a maximum matching in G equals the size of a minimum vertex cover of G.*

A connected graph G is called factor-critical if and only if $G - v$ has a perfect matching for all $v \in V(G)$. If G is a factor-critical graph, then $|V(G)| = 2\mu(G) + 1$.

Lemma 7. (Gallai Lemma) [**14**, p.84] *Let G be a connected graph. If $\mu(G - v) = \mu(G)$ for all $v \in V(G)$, then G is a factor-critical.*

Let $S_G = \{v \in V(G) : \mu(G - v) = \mu(G) - 1\}$, $D(G) = V(G) \setminus S_G$, $A(G) = \{v \in S_G : v \text{ is adjacent to a vertex in } D(G)\}$, and $C(G) = S_G \setminus A(G)$.

Theorem 8. (Edmonds-Gallai Structure Theorem) [**14**, p.93] *If G is a simple graph and $A(G), C(G)$ and $D(G)$ are defined as above, then:*

(a) the components of the graph induced by $D(G)$ are factor-critical,

(b) the subgraph induced by $C(G)$ has a perfect matching,

(c) any maximum matching of G contains a near perfect matching of $D(G)$, a perfect matching of $C(G)$ and matches all vertices of $A(G)$ with vertices in distinct components of $D(G)$.

The edge degree of an edge e is defined as the number of edges incident with e, i.e. the number of edges having common vertices with e. The maximum edge degree is denoted by Δ_e.

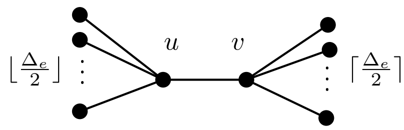

Figure 1: The graph T_1.

Lemma 9. [**18**, Theorem 1] *Let $\mathcal{T}_{\Delta_e,3}$ be the set of trees with diameter 3 and maximum edge degree Δ_e. Let $T_1 \in \mathcal{T}_{\Delta_e,3}$ be the tree as shown in Figure 1. Then for any tree $T \in \mathcal{T}_{\Delta_e,3}$, $\mathcal{E}(T) \leq \mathcal{E}(T_1)$ with equality if and only if $T = T_1$.*

Lemma 10. [**19**, Lemma 2.3] *Let T_1 be the tree depicted in Figure 1, then $\mathcal{E}(T_1) = 2\sqrt{2\Delta_e + 1}$ if Δ_e is even. $\mathcal{E}(T_1) = \sqrt{a + 2\sqrt{a}} + \sqrt{a - 2\sqrt{a}}$ with $a = 2(\Delta_e + 1)$ if Δ_e is odd.*

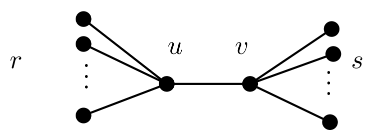

Figure 2: The graph $T_{r,s}$.

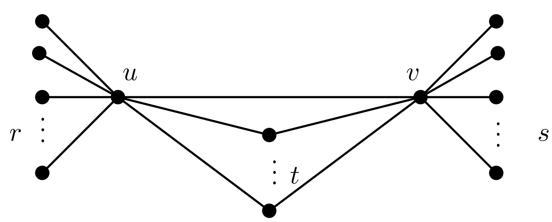

Figure 3: The graph $G_{r,s,t}$.

Let $T_{r,s}$ and $G_{r,s,t}$ stand for the graphs with structures depicted in Figures 2 and 3, respectively. The energies of $T_{r,s}$ and $G_{r,s,t}$ are related in the following way.

Lemma 11. [**17**] *For any positive integer t, $\mathcal{E}(G_{r,s,t}) < \mathcal{E}(T_{r+t,s+t})$.*

3. UPPER BOUNDS ON THE ENERGY OF GRAPHS IN TERMS OF $\mu(G)$

The following theorem was first proved for triangle free graphs in [**19**] and recently in [**17**] for any graph, not necessarily triangle free. Here we present its short proof.

Theorem 12. [**17**, Theorem 10] *Let G be a graph of order n with matching number $\mu(G)$ and maximum edge degree Δ_e. Then*

(i) if Δ_e is even, then $\mathcal{E}(G) \leq 2\mu(G)\sqrt{2\Delta_e+1}$ and equality holds if and only if G is the disjoint union of $\mu(G)$ copies of path P_2 and some isolated vertices.

(ii) if Δ_e is odd, then $\mathcal{E}(G) \leq \mu(G)(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}})$ with $a = 2(\Delta_e+1)$ and equality holds if and only if G is the disjoint union of $\mu(G)$ copies of path P_3 and some isolated vertices.

Proof: Let G be a graph of order n with matching number $\mu = \mu(G)$ and maximum edge degree Δ_e. Let $M = \{e_1, \ldots, e_\mu\}$ be a maximum matching of G. With no loss of generality, let Δ_{e_1} be the maximum value of Δ_{e_i}, $1 \leq i \leq \mu$. Let G_{e_i} be a graph containing e_i and all edges incident with e_i, $D_{e_1} = G_{e_1}$ and $D_{e_{i+1}} = G_{e_{i+1}} \setminus \bigcup_{j=1}^{i} E(D_{e_j})$ for $i \geq 1$. Since each edge out of maximum matching is incident with at least one edge in M, thus $D_{e_1}, \ldots, D_{e_\mu}$ is an edge partition of $E(G)$ and $\bigcup_{1\leq i\leq\mu} E(D_{e_i}) = E(G)$. Since for $i = 1, \ldots, \mu$, D_{e_i} are of the structure depicted in Figure 3, i.e. $D_{e_i} = G_{r_i,s_i,t_i}$ for some $r_i, t_i, s_i \geq 0$ such that $r_i + s_i + 2t_i \leq \Delta_e$, then by Lemmas 9 and 11,

$$\mathcal{E}(D_{e_i}) \leq \mathcal{E}(T_{\lfloor \frac{r_i+s_i+2t_i}{2} \rfloor, \lceil \frac{r_i+s_i+2t_i}{2} \rceil}) \leq \mathcal{E}(T_1).$$

Now, using Theorem 2 and Lemma 10, $\mathcal{E}(G) \leq \sum_{i=1}^{\mu} \mathcal{E}(T_1) = \mu\mathcal{E}(T_1)$ and so if Δ_e is even, then $\mathcal{E}(G) \leq 2\mu(G)\sqrt{2\Delta_e+1}$ and if Δ_e is odd, then $\mathcal{E}(G) \leq \mu(G)(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}})$ such that $a = 2(\Delta_e+1)$.

Now, we verify the equality case. If $\mathcal{E}(G) = \mu\mathcal{E}(T_1)$, then by Theorem 4 and Lemma 11 for $i = 1, \ldots, \mu$, $D_{e_i} = T_1$. Suppose $D_{e_1} = T_1$. If D_{e_1} is not a connected component of G, then there exists an edge e such that e meets e_1 and e_i for some i, $2 \leq i \leq \mu$, and so there exists j, $2 \leq j \leq \mu$, such that $D_{e_j} \neq T_1$, a contradiction. So, D_{e_1} is a connected component of G. If $\Delta_{e_1} \geq 2$, then by removing e_1 of M and adding two edges incident with end points of e_1, we find a matching in G larger than M, a contradiction. Thus, $\Delta_{e_1} \leq 1$. This implies that $T_1 = P_2$, if $\Delta_{e_1} = 0$ and $T_1 = P_3$ if $\Delta_{e_1} = 1$. Hence every connected component of G is P_2 if $\Delta_{e_1} = 0$ and every connected component of G is P_3 if $\Delta_{e_1} = 1$. □

Remark 13. One can easily show that if $a = 2(\Delta_e+1)$, then

$$\begin{aligned} 2\sqrt{2\Delta_e+1} &> \sqrt{2(\Delta_e+1)+2\sqrt{2(\Delta_e+1)}}+\sqrt{2(\Delta_e+1)-2\sqrt{2(\Delta_e+1)}} \\ &= \sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}}. \end{aligned}$$

By considering the 2-power of both terms in the previous inequality we obtain

$$4(2\Delta_e+1) > 4(\Delta_e+1) + 4\sqrt{\Delta_e^2-1},$$

that holds for any Δ_e.

Corollary 14. *Let G be a graph with matching number $\mu(G)$ and maximum edge degree Δ_e. Then $\mathcal{E}(G) \le 2\mu(G)\sqrt{2\Delta_e+1}$.*

Next, we aim to prove our main result: The energy of any connected graph G, with maximal vertex degree $\Delta \ge 6$ and matching number $\mu(G)$ is at most $2\mu(G)\sqrt{\Delta}$.

For the two graph classes: graphs with a perfect matching and bipartite graphs the result holds regardless of value of Δ.

Theorem 15. *If G is bipartite graph, then $\mathcal{E}(G) \le 2\mu(G)\sqrt{\Delta}$.*

Proof: Consider the vertex set of the size of the minimum vertex cover of G, $\beta(G)$, and all edges incident with these vertices. Then these edges are a partition of $E(G)$ and each of them isomorphic to $K_{1,r}$, for some r. Since $\bigcup E(K_{1,r}) = E(G)$, by Theorem 2, $\mathcal{E}(G) \le \sum \mathcal{E}(K_{1,r}) \le 2\beta(G)\sqrt{r} \le 2\beta(G)\sqrt{\Delta} = 2\mu(G)\sqrt{\Delta}$, by König's Theorem. □

Theorem 16. *Let G be a graph with maximum degree Δ which has a perfect matching. Then $\mathcal{E}(G) \le 2\mu(G)\sqrt{\Delta}$.*

Proof: By [**15**], $\mathcal{E}(G) \le \sqrt{2mn}$. On the other hand, $2m = \sum_{i=1}^{n} d_i$ such that for every $v_i \in V(G)$, $d_i = deg(v_i)$. So, $\mathcal{E}(G) \le \sqrt{(\sum_{i=1}^{n} d_i)\, n} \le \sqrt{n^2\Delta} = n\sqrt{\Delta} = 2\mu(G)\sqrt{\Delta}$. □

For graphs with largest vertex degree Δ at least 6, we first prove the following theorem.

Theorem 17. *Let G be a connected graph of order n with maximum vertex degree $\Delta = \Delta(G) \ge 6$. Then $\mathcal{E}(G) \le (n-1)\sqrt{\Delta}$.*

Proof: If $2m \le (n-2)\Delta$, then

$$\mathcal{E}(G) \le \sqrt{2mn} \le \sqrt{(n^2-n)\Delta} \le \sqrt{(n-1)^2\Delta} = (n-1)\sqrt{\Delta}.$$

Let $\alpha = \frac{2m}{n}$. Next we assume that $2m > (n-2)\Delta$, i.e., $\alpha > \frac{(n-2)\Delta}{n}$. Note also that $\alpha \le \Delta$.

By Koolen-Moulton inequality (see [**11**]) we have

$$\mathcal{E}(G) \le \alpha + \sqrt{n(n-1)\Big(\alpha - \frac{\alpha^2}{n}\Big)} = \alpha + \sqrt{(n-1)(n-\alpha)\alpha}.$$

It suffices to prove that

$$\alpha + \sqrt{(n-1)(n-\alpha)\alpha} \leq (n-1)\sqrt{\Delta}$$

or equivalently

$$(n-1)(n-\alpha)\alpha \leq (n-1)^2\Delta + \alpha^2 - 2\alpha(n-1)\sqrt{\Delta}.$$

Since $\alpha \leq \Delta$ it is enough to show that

$$(n-1)(n-\alpha) \leq (n-1)^2 + \alpha - (2n-2)\sqrt{\Delta},$$

i.e.,

$$n\alpha - n \geq (2n-2)\sqrt{\Delta} - 1.$$

Taking into account that $\alpha \geq \frac{(n-2)\Delta}{n}$, it is sufficient to prove

$$(n-2)\Delta - n \geq (2n-2)\sqrt{\Delta} - 1$$

or

$$\frac{n-2}{n-1} \geq \frac{1+2\sqrt{\Delta}}{\Delta}.$$

If $\Delta \geq 9$, then $n \geq 10$ and the previous inequality holds.

Suppose next that $6 \leq \Delta \leq 8$.

Consider the function $f(x) = x + \sqrt{(n-1)x(n-x)}$ for $x \leq \Delta$. Then

$$f'(x) = 1 + \sqrt{n-1}\frac{n-2x}{2\sqrt{x(n-x)}}.$$

If $n - 2x \geq 0$, then $f'(x) \geq 0$. Otherwise $f'(x) \geq 0$ if and only if $x \geq \frac{n}{2}$ and $2\sqrt{x(n-x)} + (n-2x)\sqrt{n-1} \geq 0$. The last one is true if and only if $x \geq \frac{n}{2}$ and $x \leq \frac{n+\sqrt{n}}{2}$. So, we conclude that $f(x)$ is an increasing function on $(0, \frac{n+\sqrt{n}}{2})$.

We differ two cases.

- If $\Delta \leq \frac{n+\sqrt{n}}{2}$, then for any $x \leq \Delta$ it follows $f(x) \leq f(\Delta)$. Our objective is to prove that $f(\Delta) \leq (n-1)\sqrt{\Delta}$ for any $\Delta \geq 6$. For this purpose we consider the following chain of equivalent inequalities.

$$\begin{aligned}
\Delta + \sqrt{(n-1)\Delta(n-\Delta)} &\leq (n-1)\sqrt{\Delta} \\
\sqrt{\Delta} + \sqrt{(n-1)(n-\Delta)} &\leq (n-1) \\
(n-1)(n-\Delta) &\leq n^2 - 2(\sqrt{\Delta}+1)n + (\sqrt{\Delta}+1)^2 \\
0 &\leq n(\Delta - 2\sqrt{\Delta} - 1) + 2\Delta + 1
\end{aligned}$$

The previous inequality holds for any n, provided that $\Delta - 2\sqrt{\Delta} - 1 \geq 0$, i.e., $\Delta \geq 6$.

- If $\Delta \geq \frac{n+\sqrt{n}}{2}$, then for any $x > 0$, $f(x) \leq f(\frac{n+\sqrt{n}}{2})$. If $\Delta = 8$, then $8 \geq \frac{n+\sqrt{n}}{2}$ implies $9 \leq n \leq 12$. If $\Delta = 7$, then $n \in \{8, 9, 10\}$, while for $\Delta = 6$, $n \in \{7, 8, 9\}$. In each case it is straightforward to verify that

$$f(\frac{n+\sqrt{n}}{2}) = \frac{n(1+\sqrt{n})}{2} \leq (n-1)\sqrt{\Delta},$$

and therefore $f(x) \leq (n-1)\sqrt{\Delta}$.

This completes the proof. □

Theorem 18. *Let G be a connected graph with maximum vertex degree $\Delta \geq 6$ and matching number $\mu(G)$. Then $\mathcal{E}(G) \leq 2\mu(G)\sqrt{\Delta}$.*

Proof: The proof goes by induction on $\mu(G)$. If $\mu(G) = 1$, then $G = S_k, k \geq 6$ (a star on $k+1$ vertices) and $\mathcal{E}(G) = 2\sqrt{k} \leq 2 \cdot 1\sqrt{\Delta}$. Next suppose that G is a graph with $\Delta \geq 6$ and matching number greater than 1.

We differ two types of connected graphs:

- Type 1: For any vertex $v \in V(G)$ the matching number of $G - v$ is equal to $\mu(G)$.
- Type 2: There exists a vertex $v \in V(G)$ such that the matching number of $G - v$ is equal to $\mu(G) - 1$.

If G is a Type 1 graph, then by Lemma 7, $n = 2\mu(G)+1$. Now the inequality holds by Theorem 17, since $\mathcal{E}(G) \leq (n-1)\sqrt{\Delta} = 2\mu(G)\sqrt{\Delta}$. If G is a Type 2 graph, then there exists a vertex v, such that the matching number of $G - v$ is equal to $\mu(G) - 1$. Let $S_G = \{v \in V(G) : \mu(G - v) = \mu(G) - 1\}$.

If there exists $v \in S_G$ such that the largest vertex degree of $G - v$, say Δ' is at least 6, then by the Induction hypothesis $\mathcal{E}(G - v) \leq 2(\mu(G) - 1)\sqrt{\Delta'}$, and consequently

$$\mathcal{E}(G) \leq \mathcal{E}(G - v) + \mathcal{E}(S_v) \leq (2\mu(G) - 2)\sqrt{\Delta} + 2\sqrt{\Delta} = 2\mu(G)\sqrt{\Delta},$$

where S_v denotes the subgraph of G that is the star with center at v and all edges incident to v.

Otherwise, for any $v \in S_G$, $\Delta(G - v) \leq 5$. Following the same notation as in Edmonds-Gallai Structure Theorem, denote by $G_1, \ldots, G_l$ distinct components of $D(G)$ and their orders by $n_1, \ldots, n_l$, respectively. Also, denote by G_C a subgraph induced by $C(G)$ and its order by n_C. By the same theorem any maximum matching of G contains a near perfect matching of $D(G)$, a perfect matching of $C(G)$ and matches all vertices of $A(G)$ with vertices in distinct components of $D(G)$. Also all G_i's are factor critical with $\Delta(G_i) = \Delta_i \leq 5$. Therefore

$$\mu(G) = \sum_{i=1}^{l} \mu(G_i) + \mu(G_C) + |A(G)|.$$

Next we show that for any G_i, $\mathcal{E}(G_i) \leq (n_i - 1)\sqrt{6}$.

Following the same lines as in the proof of Theorem 17 we obtain:

- If $\Delta_i \leq \frac{n_i + \sqrt{n_i}}{2}$, then

$$\mathcal{E}(G_i) \leq f(\Delta_i) = \Delta_i + \sqrt{\Delta_i(n_i - 1)(n_i - \Delta_i)} \leq (n_i - 1)\sqrt{6},$$

holds for any possible value of n_i.

In particular

- If $\Delta_i = 5$, then $n_i \geq 8$ and $5 + \sqrt{5(n_i - 1)(n_i - 5)} \leq (n_i - 1)\sqrt{6}$ is equivalent to $n_i^2 - (10\sqrt{6} - 18)n_i + 6 + 10\sqrt{6} \geq 0$ which is true for any $n_i \geq 8$.

- If $\Delta_i = 4$, then $n_i \geq 6$ and $4 + \sqrt{4(n_i - 1)(n_i - 4)} \leq (n_i - 1)\sqrt{6}$ is equivalent to $n_i^2 - (4\sqrt{6} - 4)n_i + 3 + 4\sqrt{6} \geq 0$ which is true for any $n_i \geq 6$.

- For $\Delta_i = 3$, we have $n_i \geq 4$ and $3 + \sqrt{3(n_i - 1)(n_i - 3)} \leq (n_i - 1)\sqrt{6}$ reduces to $n_i^2 - 2\sqrt{6}n_i + 6 + 6\sqrt{6} \geq 0$ which holds for any $n_i \geq 4$.

- For $\Delta_i = 2$, we obtain $n_i \geq 3$ and $2 + \sqrt{2(n_i - 1)(n_i - 2)} \leq (n_i - 1)\sqrt{6}$ is equivalent to $2n_i^2 - (3 + 2\sqrt{6})n_i + 6 + 4\sqrt{6} \geq 0$ which holds for any $n_i \geq 3$.

- For $\Delta_i = 1$, $1 + \sqrt{(n_i - 1)^2} \leq (n_i - 1)\sqrt{6}$ holds for any $n_i \geq 2$.

- Finally for $\Delta_i = 0$, the inequality $0 \leq (n_i - 1)\sqrt{6}$ holds for any $n_i \geq 1$.

-If $\Delta_i \geq \frac{n_i + \sqrt{n_i}}{2}$, then the order of each component is at most 7 and by Theorem 5

$$\mathcal{E}(G_i) \leq 2n_i - 2 \leq (n_i - 1)\sqrt{6}.$$

Hence, we conclude that for any component G_i of $D(G)$, $\mathcal{E}(G_i) \leq (n_i - 1)\sqrt{6}$.

Taking into account that all G_i's are factor-critical, we have that $n_i - 1 = 2\mu(G_i)$. Also, G_C has a perfect matching and by Theorem 16

$$\mathcal{E}(G_C) \leq 2\mu(G_C)\sqrt{5}.$$

If $v \in S_G$, then $v \in A(G)$ or $v \in C(G)$. If $v \in A(G)$, then

$$\begin{aligned}
\mathcal{E}(G-v) &\leq \sum_{i=1}^{l}\mathcal{E}(G_i)+\mathcal{E}(G_C)+\sum_{v'\in A(G)\setminus\{v\}}\mathcal{E}(S'_v)\\
&\leq \sum_{i=1}^{l}(n_i-1)\sqrt{6}+2\mu(G_C)\sqrt{5}+2(|A(G)|-1)\sqrt{\Delta}\\
&\leq \sum_{i=1}^{l}2\mu(G_i)\sqrt{6}+2\mu(G_C)\sqrt{6}+2(|A(G)|-1)\sqrt{\Delta}\\
&\leq 2\Big(\sum_{i=1}^{l}\mu(G_i)+\mu(G_C)+|A(G)|-1\Big)\sqrt{\Delta}\\
&= 2(\mu(G)-1)\sqrt{\Delta}.
\end{aligned}$$

If $v\in C(G)$, then $\mu(G_C-v)=\mu(G_C)-1$, taking into account that G_C has a perfect matching. Similarly as for G_i's we conclude that $\mathcal{E}(G_C-v)\leq(n_C-2)\sqrt{6}$, since the order of G_C-v is n_C-1 and the largest vertex degree is at most 5. As a result we have

$$\begin{aligned}
\mathcal{E}(G-v) &\leq \sum_{i=1}^{l}\mathcal{E}(G_i)+\mathcal{E}(G_C-v)+\sum_{v'\in A(G)}\mathcal{E}(S'_v)\\
&\leq \sum_{i=1}^{l}(n_i-1)\sqrt{6}+(n_C-2)\sqrt{6}+2|A(G)|\sqrt{\Delta}\\
&\leq \sum_{i=1}^{l}2\mu(G_i)\sqrt{6}+2(\mu(G_C)-1)\sqrt{6}+2|A(G)|\sqrt{\Delta}\\
&\leq 2\Big(\sum_{i=1}^{l}\mu(G_i)+\mu(G_C)-1+|A(G)|\Big)\sqrt{\Delta}\\
&= 2(\mu(G)-1)\sqrt{\Delta}.
\end{aligned}$$

Next,

$$\mathcal{E}(G)\leq\mathcal{E}(G-v)+\mathcal{E}(S_v)\leq 2(\mu(G)-1)\sqrt{\Delta}+2\sqrt{\Delta}=2\mu(G)\sqrt{\Delta}.$$

This completes the proof. □

Remark 19. The bound obtained in Theorem 18 improves the bound proven in Theorem 12, $\mathcal{E}(G)\leq 2\mu(G)\sqrt{2\Delta_e+1}$ for connected graphs, since $2\Delta_e+1\geq\Delta$. Moreover, $\Delta_e\geq\Delta$. Recall, Δ_e denotes the maximum edge degree.

Corollary 20. *Let G be a r-regular graph, $r\geq 6$ with matching number $\mu(G)$, then $\mathcal{E}(G)\leq 2\mu(G)\sqrt{r}$.*

Experimental results suggest that $\mathcal{E}(G) \leq 2\mu(G)\sqrt{\Delta}$ holds for any graph $G \neq C_3, C_5, C_9$. Using the same approach as in Theorem 17 it can be verified that if $\Delta \leq \frac{n+\sqrt{n}}{2}$ and $\Delta = 5$, then $f(\Delta) \leq (n-1)\sqrt{\Delta}$ for any $n \in \{6, 7, 8, 9, 10, 11\}$, while for $\Delta = 4$ it holds for $n = 5$. If $\Delta \geq \frac{n+\sqrt{n}}{2}$ and $\Delta \in \{2, 3, 4, 5\}$ the inequality $f(\Delta) \leq (n-1)\sqrt{\Delta}$ holds for any possible value of n. Therefore it remains to verify that the bound holds for $\Delta = 5, n \geq 12$, $\Delta = 4, n \geq 6$, $\Delta = 3, n \geq 4$ and $\Delta = 2, n \geq 3$ assuming that $G \neq C_3, C_5, C_9$.

4. SOME RELATED OPEN PROBLEMS

It remains unanswered which of the graphs $G_{r,s,t}$ of fixed order n has maximum energy. According to numerical results we obtained, we conjecture the following.

Conjecture 21. *In the class of all graphs $G_{r,s,t}$, $0 \leq r, s, t \leq n$ of fixed order $n = r + s + t + 2$ the graph G_{r_0,s_0,t_0} with maximum energy is:*

$$G_{r_0,s_0,t_0} = \begin{cases} G_{k,k-1,4k-1}, & \textit{if} \quad n = 6k; \\ G_{k,k-1,4k}, & \textit{if} \quad n = 6k+1; \\ G_{k,k,4k}, & \textit{if} \quad n = 6k+2; \\ G_{k,k,4k+1}, & \textit{if} \quad n = 6k+3; \\ G_{k,k,4k+2}, & \textit{if} \quad n = 6k+4; \\ G_{k+1,k,4k+2}, & \textit{if} \quad n = 6k+5. \end{cases}$$

Here we present some partial results obtained in an attempt to determine an energy maximizer.

It is easy to observe that the vertex set $V(G_{r,s,t})$ admits an equitable partition $V(G_{r,s,t}) = \{X_1, X_2, X_3, X_4, X_5\}$, where X_1 and X_5 contain all pendant vertices adjacent to u, v respectively, $X_2 = \{u\}$, $X_4 = \{v\}$ and X_3 is the set of all vertices of degree 2. Thus, it follows that the quotient matrix B of $A_{G_{r,s,t}}$ is

$$B = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ r & 0 & t & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & t & 0 & s \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

We obtain that the characteristic polynomial of B equals to

$$\varphi_B(x) = x^5 - (r + s + 2t + 1)x^3 - 2tx^2 + (rs + rt + st)x$$

and by Lemma 1, all the nonzero eigenvalues of $A_{G_{r,s,t}}$ are the eigenvalues of B. In particular, we also conclude that

$$\varphi_{A_{G_{r,s,t}}}(x) = x^{n-4}(x^4 - (r + s + 2t + 1)x^2 - 2tx + (rs + rt + st)).$$

If $r = s$, then

$$(1)\qquad \begin{aligned} & x^4-(r+s+2t+1)x^2-2tx+(rs+rt+st) \\ = \;& x^4-(2s+2t+1)x^2-2tx+(s^2+2st) \\ = \;& (x^2-x-s-2t)(x^2+x-s). \end{aligned}$$

By the Coulson integral formula, we obtain

$$\begin{aligned} \mathcal{E}(G_{r,s,t}) &= \frac{1}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln\left[(b_0+b_2x^2+b_4x^4)^2+(b_3x^3)^2\right]dx \\ (2)\qquad &= \frac{1}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln\left[(1+(r+s+2t+1)x^2+(rs+rt+st)x^4)^2+(2tx^3)^2\right]dx \end{aligned}$$

Regarding the energy of $G_{r,s,t}$ we prove the following claims.

Claim 1. For any $t \le n-2$,

$$\mathcal{E}(G_{r,s,t}) \le \mathcal{E}(G_{\lfloor \frac{r+s}{2}\rfloor,\lceil \frac{r+s}{2}\rceil,t}).$$

Proof: By (2) $\mathcal{E}(G_{\lfloor \frac{r+s}{2}\rfloor,\lceil \frac{r+s}{2}\rceil,t})$ equals to

$$\frac{1}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln\left[(1+(r+s+2t+1)x^2+(\lfloor\frac{r+s}{2}\rfloor\lceil\frac{r+s}{2}\rceil+(r+s)t)x^4)^2+(2tx^3)^2\right]dx.$$

For any r,s,t and $i \in \{0,2,3\}$,

$$b_i(G_{\lfloor \frac{r+s}{2}\rfloor,\lceil \frac{r+s}{2}\rceil,t}) = b_i(G_{r,s,t}),$$

while

$$b_4(G_{\lfloor \frac{r+s}{2}\rfloor,\lceil \frac{r+s}{2}\rceil,t}) \ge b_4(G_{r,s,t}).$$

This proves our claim. □

Claim 2. If $t \le n-2$ and $n-t$ is even, then

$$\mathcal{E}(G_{r,s,t}) \le \mathcal{E}(G_{\frac{n-t-2}{2},\frac{n-t-2}{2},t})$$

Also,

$$\mathcal{E}(G_{r,s,t}) \le \begin{cases} \mathcal{E}(G_{k,k,4k-2}) = \sqrt{4k+1}+\sqrt{36k-15}, & \text{if} \quad n=6k; \\ \mathcal{E}(G_{k,k,4k-1}) = \sqrt{4k+1}+\sqrt{36k-7}, & \text{if} \quad n=6k+1; \\ \mathcal{E}(G_{k,k,4k}) = \sqrt{4k+1}+\sqrt{36k+1}, & \text{if} \quad n=6k+2; \\ \mathcal{E}(G_{k,k,4k+1}) = \sqrt{4k+1}+\sqrt{36k+9}, & \text{if} \quad n=6k+3; \\ \mathcal{E}(G_{k,k,4k+2}) = \sqrt{4k+1}+\sqrt{36k+17}, & \text{if} \quad n=6k+4; \\ \mathcal{E}(G_{k,k,4k+3}) = \sqrt{4k+1}+\sqrt{36k+25}, & \text{if} \quad n=6k+5. \end{cases}$$

Proof: According to (1) in case when $r = s$ we can calculate all nonzero eigenvalues of $G_{s,s,t}$ and find that

$$\mathcal{E}(G_{s,s,t}) = \sqrt{1+4s} + \sqrt{1+4s+2t}.$$

Bearing in mind that $2s = n - t - 2$, we obtain that $\mathcal{E}(G_{s,s,t})$ can be seen as a function of t, i.e.,

$$\mathcal{E}(G_{\frac{n-t-2}{2},\frac{n-t-2}{2},t}) = g(t) = \sqrt{2n-2t-3} + \sqrt{2n+6t-3}.$$

We look for the maximum of this function. Taking into account that $g'(t) > 0$ if and only if $t < \frac{2}{3}n - 1$, we differ the following cases regarding $(n \mod 6)$.

i) If $n = 6k$ for some $k \geq 1$, then the maximum is attained either at $t = 4k - 2$ or at $t = 4k$, since $\frac{2}{3}n - 1 = 4k - 1$ and $n - (4k - 1)$ is not even. By direct computation we verify, that $g(4k-2) > g(4k)$.

ii) If $n = 6k + 1$ for some $k \geq 1$, then $\frac{2}{3}n - 1 = 4k - \frac{1}{3}$, so the maximum is attained either at $4k - 1$ or at $4k + 1$, since $n - 4k$ is odd. Direct computation shows that the maximum is at $4k - 1$.

iii) If $n = 6k + 2$ for some $k \geq 1$, then $\frac{2}{3}n - 1 = 4k + \frac{1}{3}$. Similarly as in the previous case we conclude that the maximum is attained at $4k$.

iv) In same fashion it follows that if $n = 6k + 3$ for some $k \geq 0$, the maximum is attained at $4k + 1$.

v) If $n = 6k + 4$ for some $k \geq 0$, then the maximum is attained at $4k + 2$.

vi) If $n = 6k + 5$ for some $k \geq 0$, then the maximum is attained at $4k + 3$.

□

Claim 3. Let G_{s_0+1,s_0,t_0} be the graph with maximal energy among graphs $G_{r,s,t}$ such that $n - t$ is odd. Then

$$\mathcal{E}(G_{s_0+1,s_0,t_0}) \leq \begin{cases} \mathcal{E}(G_{k,k,4k-1}) = \sqrt{4k+1} + \sqrt{36k-7}, & \text{if} \quad n = 6k; \\ \mathcal{E}(G_{k,k,4k}) = \sqrt{4k+1} + \sqrt{36k+1}, & \text{if} \quad n = 6k+1; \\ \mathcal{E}(G_{k,k,4k+1}) = \sqrt{4k+1} + \sqrt{36k+9}, & \text{if} \quad n = 6k+2; \\ \mathcal{E}(G_{k,k,4k+2}) = \sqrt{4k+1} + \sqrt{36k+17}, & \text{if} \quad n = 6k+3; \\ \mathcal{E}(G_{k,k,4k+3}) = \sqrt{4k+1} + \sqrt{36k+25}, & \text{if} \quad n = 6k+4; \\ \mathcal{E}(G_{k+1,k+1,4k+2}) = \sqrt{4k+5} + \sqrt{36k+21}, & \text{if} \quad n = 6k+5 \end{cases}$$

and

$$\mathcal{E}(G_{s_0+1,s_0,t_0}) \geq \begin{cases} \mathcal{E}(G_{k-1,k-1,4k-1}) = \sqrt{4k-3} + \sqrt{36k-11}, & \text{if} \quad n = 6k; \\ \mathcal{E}(G_{k,k,4k-2}) = \sqrt{4k-1} + \sqrt{36k-17}, & \text{if} \quad n = 6k+1; \\ \mathcal{E}(G_{k,k,4k-1}) = \sqrt{4k+1} + \sqrt{36k-7}, & \text{if} \quad n = 6k+2; \\ \mathcal{E}(G_{k,k,4k}) = \sqrt{4k+1} + \sqrt{36k+1}, & \text{if} \quad n = 6k+3; \\ \mathcal{E}(G_{k,k,4k+1}) = \sqrt{4k+1} + \sqrt{36k+9}, & \text{if} \quad n = 6k+4; \\ \mathcal{E}(G_{k,k,4k+2}) = \sqrt{4k+1} + \sqrt{36k+17}, & \text{if} \quad n = 6k+5. \end{cases}$$

Proof: For any t, such that $n-t$ is odd, the graph with the maximal energy is $G_{\frac{n-t-3}{2},\frac{n-t-1}{2},t}$. Also by Coulson integral formula it follows

$$\mathcal{E}(G_{\frac{n-t-3}{2},\frac{n-t-3}{2},t}) \leq \mathcal{E}(G_{\frac{n-t-3}{2},\frac{n-t-1}{2},t}) \leq \mathcal{E}(G_{\frac{n-t-1}{2},\frac{n-t-1}{2},t}).$$

We consider only the case $n = 6k$. The other cases are proven in a similar way. According to Claim 2,

$$\mathcal{E}(G_{\frac{n-t-1}{2},\frac{n-t-1}{2},t}) \leq \mathcal{E}(G_{k,k,4k-1}),$$

since $G_{\frac{n-t-1}{2},\frac{n-t-1}{2},t}$ is of the order $6k+1$.

By taking maximum over all $t \leq n-2$, such that $n-t$ is odd, from

$$\mathcal{E}(G_{\frac{n-t-3}{2},\frac{n-t-3}{2},t}) \leq \mathcal{E}(G_{\frac{n-t-3}{2},\frac{n-t-1}{2},t})$$

we obtain

$$\mathcal{E}(G_{k-1,k-1,4k-1}) \leq \mathcal{E}(G_{s_0+1,s_0,t_0}),$$

again by Claim 2.

□

Remark 22. By Claims 2 and 3 it follows that for n sufficiently large the maximal energy of $G_{r,s,t}$ asymptotically behaves as $8\sqrt{\lfloor \frac{n}{6} \rfloor}$.

We end the paper with the conjecture on the remaining, uncovered cases from Theorem 18.

Conjecture 23. *For any graph $G \neq C_3, C_5, C_7$, with the matching number $\mu(G)$ and the largest vertex degree $\Delta \in \{2,3,4,5\}$, $\mathcal{E}(G) \leq 2\mu(G)\sqrt{\Delta}$.*

Acknowledgements. We thank Fatemah Koorepazan-Moftakhar for her fruitful comments. This work was supported by Kuwait University, Research Grant No. SM02/19.

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(Received 27. 12. 2020.)
(Revised 18. 04. 2021.)

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