MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **83** (2020) 541-554

ISSN 0340 - 6253

Upper Bounds of Graph Energy in Terms of Matching Number

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(Received May 3, 2019)

Abstract

The energy of a graph G, denoted by $\mathcal{E}(G)$, is the sum of the absolute values of all the eigenvalues of its adjacency matrix $A(G)$. In this paper, we give the upper bounds of graph energy in terms of matching number and characterize all the extremal graphs achieving the upper bounds.

1 Introduction

Graphs considered in this paper are simple and undirected. For a graph G, let $V(G)$ and $E(G)$ denote the vertex set and edge set of G, respectively. For an edge e of G, the *edge degree* $d(e)$ is the number of edges incident with e. The *maximum edge degree* of G is denoted by $\Delta_e(G)$. Without confusion, we denote $\Delta_e(G)$ by Δ_e. An edge set M of G is called a *matching* if any two edges in M have no common vertices. If a matching M of G contains k edges, then it is called a *k-matching*. Given an n-vertex graph G, the number of k-matchings in G is denoted by $m(G,k)$ and in particular $m(G,0)=1$. If each vertex of G is incident with exactly one edge of M, then M is called a *perfect matching* of G. The *matching number* of a graph G, denoted by $\mu(G)$, is the number of edges in

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a maximum matching. For any two vertex-disjoint graphs G and H, the *union* $G \cup H$ is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. The complete graph of order n is denoted by K_n, and in particular, K_1 denotes the trivial graph with exactly one vertex. In this paper, tG denotes the union of t graph G.

The *graph energy* $\mathcal{E}(G)$ of G, proposed by Gutman [9], is the sum of the absolute values of all the eigenvalues of the adjacency matrix $A(G)$, i.e. $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $A(G)$. Obviously, isolated vertices have no influence on the energy of a graph.

The theory of graph energy is well developed nowadays. For detailed results on graph energy, we refer the reader to the book [14]. In this article, we are interested in the upper bounds of the graph energy of G. McClelland [15] proved that $\mathcal{E}(G) \leq \sqrt{2mn}$ for any graph G with n vertices and m edges, moreover, if G is a connected non-singular graph, Das and Gutman [5] proved that $\mathcal{E}(G) \leq 2m - \frac{2m}{n}(\frac{2m}{n} - 1) - \ln(\frac{n|\det \mathbf{A}|}{2m})$, where $\det \mathbf{A}$ is the determinant of the adjacency matrix $A(G)$. For a graph G with vertex cover number τ and maximum degree Δ, Wang and Ma [20] proved that $\mathcal{E}(G) \leq 2\tau\sqrt{\Delta}$. Das and Mojallal [4] presented some new upper bounds for $\mathcal{E}(G)$ in terms of the number of vertices or edges, clique number, minimum degree, and the first Zagreb index. Rada and Tineo [16] gave the upper bounds of the energy of a bipartite graph using the graph order, size and the spectral moment of fourth order. Hou et al. [11] established a upper bound for the energy of a graph by considering a new lower bound of spectral radius. Alawiah et al. [1] obtained various new upper bounds for the energy of graphs in terms of the graph order, size, maximum degree, and the first Zagreb index, which improved several previous bounds given in [12, 13, 15].

Recently, many researchers pay attention to the relation between the energy of a graph G and the matching number $\mu(G)$ of G. Ashraf [2] investigated the energy of trees with perfect matching. Wong et al. [19] gave lower bounds of graph energy in terms of matching number such that $\mathcal{E}(G) \geq 2\mu(G)$. Tian and Wong [18] established the upper bounds of the energy for triangle-free graphs in terms of matching number. Thus, it makes sense to give the upper bounds of the energy of general graphs in terms of matching number.

In this paper, we investigate the upper bounds of graph energy in terms of matching number in Section 3 and determine the corresponding extremal graphs attaining the upper bound in Section 4.

Theorem 1. *Let G be an n-vertex graph with matching number $\mu(G)$ and maximum edge degree Δ_e.*

(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 $G \cong \mu(G)P_2 \cup (n - 2\mu(G))K_1$.*

(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 $G \cong \mu(G)P_3 \cup (n - 3\mu(G))K_1$.*

2 Preliminaries

Let G be a simple n-vertex graph. The *characteristic polynomial* $\phi(G)$ of G is defined as $\phi(G) = \det(xI - A(G))$, where I is an identity matrix of order n. The *matching polynomial* $\alpha(G)$ of G is defined as

$$\alpha(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(G,k) x^{n-2k}.$$

Godsil and Gutman [8] determined the relation between the matching polynomial $\alpha(G)$ and the characteristic polynomial $\phi(G)$ of a graph G as follows.

Lemma 2. *[8] Let $\phi(G)$ denote the characteristic polynomial of G. Then $\phi(G) = \alpha(G) + \sum_C (-2)^{t(C)} \alpha(G - C)$, where the summation is over all nontrivial subgraphs C of G which are unions of vertex-disjoint cycles and $t(C)$ is the number of components of C, where $G - C$ denotes the graph by deleting the vertices in C from G.*

Lemma 3. *[8] The matching polynomial of a graph coincides with the characteristic polynomial if and only if the graph is a forest.*

Coulson [3] studied the energy of chemical molecules and obtained a classical Coulson integral formula which presents the relation between the energy and the characteristic polynomial of graphs. The graph energy $\mathcal{E}(G)$ can be expressed as the Coulson integral formula (see [10])

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

where the characteristic polynomial of G is $\phi(G) = a_0 x^n + a_1 x^{n-1} + \cdots + a_n$.

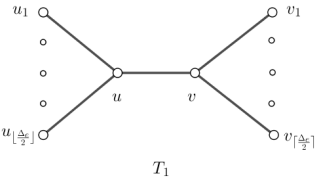

Figure 1. Graph T_1

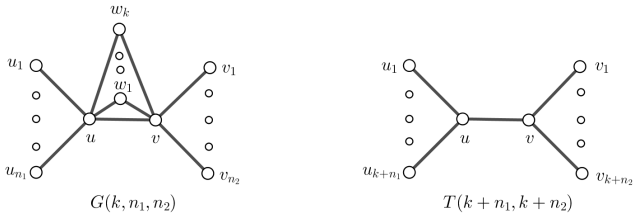

Figure 2. Graphs $G(k, n_1, n_2)$ and $T(k + n_1, k + n_2)$.

Let $\mathcal{T}_{\Delta_e,3}$ denote the set of trees with diameter 3 and maximum edge degree Δ_e. Denote the tree shown in Figure 1 by T_1, which is a graph in $\mathcal{T}_{\Delta_e,3}$. Renqian et al. [17] considered the energy of the trees in $\mathcal{T}_{\Delta_e,3}$ and obtained the following result.

Lemma 4. *[17] For any tree $T \in \mathcal{T}_{\Delta_e,3}$, $\mathcal{E}(T) \leq \mathcal{E}(T_1)$ and equality holds if and only if $T = T_1$.*

In order to calculate the energy for triangle-free graphs, Tian and Wong [18] gave the exact value of $\mathcal{E}(T_1)$ as follows.

Lemma 5. *[18] For any positive integer Δ_e, $\mathcal{E}(T_1) = 2\sqrt{2\Delta_e + 1}$ 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.*

Let k be a positive integer, and let n_1, n_2 be two non-negative integers. Let $G(k, n_1, n_2)$ and $T(k+n_1, k+n_2)$ be two connected graphs as shown in Figure 2. The relation between the energy of $G(k, n_1, n_2)$ and that of $T(k + n_1, k + n_2)$ is obtained as follows.

Lemma 6. *For any positive integer k, $\mathcal{E}(G(k, n_1, n_2)) < \mathcal{E}(T(k + n_1, k + n_2))$.*

Proof. Let $s = 2k + n_1 + n_2$, then $s \geq 2$. Let $G_1(k, n_1, n_2) = G(k, n_1, n_2) \cup kK_1$, then $|V(G_1(k, n_1, n_2))| = |V(T(k + n_1, k + n_2))| = s + 2$. Since

$$\mathcal{E}(G(k, n_1, n_2)) = \mathcal{E}(G_1(k, n_1, n_2)),$$

then we only need to prove that

$$\mathcal{E}(G_1(k, n_1, n_2)) < \mathcal{E}(T(k + n_1, k + n_2)).$$

By Lemma 3, we have

$$\phi(T(k+n_1, k+n_2)) = \alpha(T(k+n_1, k+n_2)) = x^{s+2} - (s+1)x^s + (k^2 + kn_1 + kn_2 + n_1n_2)x^{s-2}.$$

Moreover, by Lemma 2,

$$\begin{aligned}
\phi(G_1(k, n_1, n_2)) &= \alpha(G_1(k, n_1, n_2)) + \sum_{C} (-2)^{t(C)} \alpha(G_1(k, n_1, n_2) - C) \\
&= \alpha(G_1(k, n_1, n_2)) - 2\sum_{j=1}^{k} \alpha(G_1(k, n_1, n_2) - uvw_j) \\
&\quad - 2 \sum_{1 \leq i < j \leq k} \alpha(G_1(k, n_1, n_2) - uw_ivw_j) \\
&= x^{s+2} - (s+1)x^s + (n_1n_2 + kn_1 + kn_2)x^{s-2} - 2k\alpha((s-1)K_1) \\
&\quad - k(k-1)\alpha((s-2)K_1) \\
&= x^{s+2} - (s+1)x^s - 2kx^{s-1} + (n_1n_2 + kn_1 + kn_2 - k^2 + k)x^{s-2}.
\end{aligned}$$

By the Coulson integral formula (1), it can be obtained that

$$\mathcal{E}(T(k + n_1, k + n_2)) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln f(x, s) dx$$

and

$$\mathcal{E}(G_1(k, n_1, n_2)) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln g(x, s) dx,$$

where

$$f(x, s) = \left(1 + (s+1)x^2 + (k^2 + kn_1 + kn_2 + n_1n_2)x^4\right)^2,$$

$$g(x, s) = \left(1 + (s+1)x^2 + (n_1n_2 + kn_1 + kn_2 - k^2 + k)x^4\right)^2 + (2kx^3)^2.$$

Moreover,

$$f(x, s) - g(x, s) = (2k^2 - k)x^4 \cdot \left(2 + 2(s+1)x^2 + (2n_1n_2 + 2kn_1 + 2kn_2 + k)x^4\right)$$

$$
\begin{aligned}
&- 4k^2x^6 \geq k^2x^4 \cdot \Big(2 + 2(s+1)x^2 + (2n_1n_2 + 2kn_1 + 2kn_2 + k)x^4\Big) \\
&- 4k^2x^6 = k^2x^4 \cdot \Big(2 + 2(s-1)x^2 + (2n_1n_2 + 2kn_1 + 2kn_2 + k)x^4\Big) \\
&\geq 0.
\end{aligned}
$$

and equality holds if and only if $x = 0$. Hence, $\mathcal{E}(G_1(k, n_1, n_2)) < \mathcal{E}(T(k + n_1, k + n_2))$, and thus, $\mathcal{E}(G(k, n_1, n_2)) < \mathcal{E}(T(k + n_1, k + n_2))$. ■

A graph H is called an induced subgraph of graph G if H is obtained from G by deleting some vertices along with all edges incident with them. If H is an induced subgraph of G, the relation between $\mathcal{E}(G)$ and $\mathcal{E}(H)$ is given below.

Lemma 7. *[6] Let H be an induced subgraph of G. Then $\mathcal{E}(H) \leq \mathcal{E}(G)$ with equality holds if and only if each edge of G is also an edge of H.*

Let T_1 and $G(k, n_1, n_2)$ denote the graphs which are shown in Figure 1 and 2, respectively. Remind that the maximum edge degree of T_1 is denoted by Δ_e. The relation of the graph energies for T_1 and $G(k, n_1, n_2)$ are given below.

Lemma 8. *For any positive integer k and non-negative integers n_1 and n_2, if $2k+n_1+n_2 \leq \Delta_e$, then $\mathcal{E}(G(k, n_1, n_2)) < \mathcal{E}(T_1)$.*

Proof. Since $2k + n_1 + n_2 \leq \Delta_e$, then we can construct a tree T_2 with diameter 3 and maximum edge degree Δ_e such that $T(k + n_1, k + n_2)$ is an induced subgraph of T_2. By Lemma 7, we have $\mathcal{E}(T(k + n_1, k + n_2)) \leq \mathcal{E}(T_2)$. Together with Lemma 4 and Lemma 6, we have

$$\mathcal{E}(G(k, n_1, n_2)) < \mathcal{E}(T(k + n_1, k + n_2)) \leq \mathcal{E}(T_2) \leq \mathcal{E}(T_1)$$

as desired. ■

Lemma 9. *[7] Let X, Y, Z be real symmetric matrices of order n such that $Z = X + Y$. Then $\mathcal{E}(Z) \leq \mathcal{E}(X) + \mathcal{E}(Y)$.*

3 Upper bounds of graph energy

Let G be a simple graph. In this section, we will give the upper bound of the graph energy of G in terms of matching number. Let $G - e$ denote the graph obtained from G by deleting an edge $e \in E(G)$ and also its two endpoints.

Theorem 10. *Let G be an n-vertex graph with matching number $\mu(G)$ and maximum edge degree Δ_e, then the graph energy $\mathcal{E}(G)$ is shown as below:*

(i) *If Δ_e is even, then $\mathcal{E}(G) \leq 2\mu(G)\sqrt{2\Delta_e + 1}$.*

(ii) *If Δ_e is odd, then $\mathcal{E}(G) \leq \mu(G)(\sqrt{a + 2\sqrt{a}} + \sqrt{a - 2\sqrt{a}})$ with $a = 2(\Delta_e + 1)$.*

Proof. We complete the proof by applying the induction on the matching number $\mu(G)$. Moreover, we only give the proof for the case when Δ_e is even. The case for which Δ_e is odd can be proved similarly. Assume now that Δ_e is even. If $\mu(G) = 1$, then $G \cong C_3 \cup (n-3)K_1$ or $G \cong S_k \cup (n-k)K_1$, where $2 \leq k \leq n$ and k is even. If $G \cong C_3 \cup (n-3)K_1$, then $\Delta_e = 2$ and

$$\mathcal{E}(G) = 4 < 2\sqrt{5} = 2\mu(G)\sqrt{2\Delta_e + 1}.$$

If $G \cong S_k \cup (n-k)K_1$ ($2 \leq k \leq n$ and k is even), then $\Delta_e = k - 2$ and

$$\mathcal{E}(G) = 2\sqrt{k-1} \leq 2\sqrt{2k-3} = 2\mu(G)\sqrt{2\Delta_e + 1}.$$

Let μ be an integer such that $\mu \geq 2$. For any graph H with even maximum edge degree $\Delta_e(H)$ and matching number $\mu(H) < \mu$, suppose that $\mathcal{E}(H) \leq 2\mu(H)\sqrt{2\Delta_e(H) + 1}$. For the graph G with $\mu(G) = \mu$, let M be a maximum matching of G and let $e_{uv} := uv$ be an edge of M, where u and v are the endpoints of e_{uv}. Then the adjacency matrix $A(G)$ of G can be rewritten as in which the first two rows and columns are indexed by u and v, respectively:

$$A(G) = \begin{pmatrix} 0 & 1 & \alpha^t \\ 1 & 0 & \beta^t \\ \alpha & \beta & A(G - e_{uv}) \end{pmatrix},$$

where α, β are two column vectors, and $A(G - e_{uv})$ is the adjacency matrix of the graph $G - e_{uv}$. Obviously,

$$A(G) = \begin{pmatrix} 0 & 1 & \alpha^t \\ 1 & 0 & \beta^t \\ \alpha & \beta & \mathbf{0} \end{pmatrix} + \begin{pmatrix} 0 & 0 & \mathbf{0} \\ 0 & 0 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & A(G - e_{uv}) \end{pmatrix}.$$

Let G_0 be a graph whose adjacency matrix is $\begin{pmatrix} 0 & 1 & \alpha^t \\ 1 & 0 & \beta^t \\ \alpha & \beta & \mathbf{0} \end{pmatrix}$. Then by Lemma 9,

$$\mathcal{E}(G) \leq \mathcal{E}(G_0) + \mathcal{E}(G - e_{uv}). \tag{2}$$

We now give the following two claims about the energy of G_0 and $G - e_{uv}$.

Claim 1: $\mathcal{E}(G_0) \leq 2\sqrt{2\Delta_e + 1}$.

We complete the proof of Claim 1 according to all the possibilities of G_0. If $G_0 \cong S_k \cup (n-k)K_1$ $(k \geq 2)$, then $\Delta_e \geq \Delta_e(G_0) = k - 2$ and thus

$$\mathcal{E}(G_0) = 2\sqrt{k-1} \leq 2\sqrt{2k-3} \leq 2\sqrt{2\Delta_e + 1}.$$

If $G_0 \cong T \cup (n-k)K_1$ $(k \geq 4)$, where T is a k-vertex tree with diameter 3 and maximum edge degree $\Delta_e(T) \leq \Delta_e$, then $\mathcal{E}(G_0) = \mathcal{E}(T)$ and we can find a tree T_0 with diameter 3 and maximum edge degree Δ_e such that T is a subgraph of T_0. By Lemma 7, we have $\mathcal{E}(T) \leq \mathcal{E}(T_0)$. By Lemma 4, we have

$$\mathcal{E}(G_0) = \mathcal{E}(T) \leq \mathcal{E}(T_0) \leq \mathcal{E}(T_1) = 2\sqrt{2\Delta_e + 1}.$$

If $G_0 \cong G(k, n_1, n_2) \cup (n - n_1 - n_2 - k - 2)K_1$ $(k \geq 1, n_1 \geq 0, n_2 \geq 0, n_1 + n_2 + k + 2 \leq n)$, since $\Delta_e(G_0) = 2k + n_1 + n_2 \leq \Delta_e$, by Lemma 8, we have

$$\mathcal{E}(G_0) = \mathcal{E}(G(k, n_1, n_2)) < \mathcal{E}(T_1) = 2\sqrt{2\Delta_e + 1}.$$

Thus, for each possibility of G_0 listed above, $\mathcal{E}(G_0) \leq 2\sqrt{2\Delta_e + 1}$ if Δ_e is even.

Claim 2: $\mathcal{E}(G - e_{uv}) \leq 2(\mu(G) - 1)\sqrt{2\Delta_e + 1}$.

It is obvious that $M - e_{uv}$ is a maximum matching of $G - e_{uv}$ and so $\mu(G - e_{uv}) = \mu(G) - 1$. Since $\Delta_e(G - e_{uv}) \leq \Delta_e$, by induction, we have

$$\mathcal{E}(G - e_{uv}) \leq 2(\mu(G) - 1)\sqrt{2\Delta_e(G - e_{uv}) + 1} \leq 2(\mu(G) - 1)\sqrt{2\Delta_e + 1}.$$

By Claim 1 and Claim 2, we have $\mathcal{E}(G) \leq 2\mu(G)\sqrt{2\Delta_e + 1}$ if Δ_e is even. ■

Remark 1. Consider the graph $G(k, n_1, n_2)$ as shown in Figure 2. Then $n = n_1 + n_2 + k + 2$ and $m = n_1 + n_2 + 2k + 1$, where n and m denote the sizes of the vertex set and edge set of the graph $G(k, n_1, n_2)$, respectively. If $\Delta_e = n_1 + n_2 + 2k$ is even, then $\mathcal{E}(G(k, n_1, n_2)) \leq 4\sqrt{2n + 2k - 3}$. For $n \geq 16$, $\mathcal{E}(G(k, n_1, n_2)) \leq 4\sqrt{2n + 2k - 3} < \sqrt{2(n + k - 1)n} = \sqrt{2mn}$, which is the bound obtained in [15].

4 Extremal graphs

In this section, we will characterize all extremal graphs achieving the upper bounds. Let G be an extremal graph with maximum edge degree Δ_e and matching number $\mu(G)$. As given in Section 3, let M denote a maximum matching of G and let $e_{uv} := uv$ be an edge of M.

Lemma 11. *Let $d(e')$ denote the edge degree of any edge $e' \in M$, then $d(e') = \Delta_e$.*

Proof. If Δ_e is even, since G is a graph with $\mathcal{E}(G) = 2\mu(G)\sqrt{2\Delta_e + 1}$, by the investigation of the energy of the graph G_0 in Claim 1, we have $\mathcal{E}(G_0) = 2\sqrt{2\Delta_e + 1}$ and moreover, $G_0 \cong T_1 \cup (n - \Delta_e - 2)K_1$ or $G_0 \cong S_2 \cup (n-2)K_1$, $\Delta_e(G_0) = \Delta_e$. Thus, $d(e_{uv}) = \Delta_e$. By the arbitrariness of the edge $e_{uv} \in M$, $d(e') = \Delta_e$ for any edge $e' \in M$. If Δ_e is odd, the result can be proved Similarly. ■

For the graph G and its maximum matching M, let $G - ke$ denote the graph obtained by removing k $(1 \leq k \leq \mu(G))$ edges together with their endpoints of M from G. Let $\mu(G - ke)$ denote the matching number of the graph $G - ke$. Similar to the proof of the Claim 2 in the paper [18], the following result holds.

Lemma 12. *For the graph G whose energy attains the upper bound in Theorem 10, the following results hold:*

(i) *If Δ_e is even, then $\mathcal{E}(G - ke) = 2\mu(G - ke)\sqrt{2\Delta_e + 1}$.*

(ii) *If Δ_e is odd, then $\mathcal{E}(G-ke) = \mu(G-ke)(\sqrt{a + 2\sqrt{a}} + \sqrt{a - 2\sqrt{a}})$ with $a = 2(\Delta_e+1)$.*

Proof. Assume first that Δ_e is even. Let G be a graph with $\mathcal{E}(G) = 2\mu(G)\sqrt{2\Delta_e + 1}$ and let M be its maximum matching. Since $\mathcal{E}(G) = 2\mu(G)\sqrt{2\Delta_e + 1}$, by the investigation of Claim 2, for the edge $e_{uv} := uv$ of M, we have $\mathcal{E}(G - e_{uv}) = 2(\mu(G) - 1)\sqrt{2\Delta_e + 1}$ and $\Delta_e(G - e_{uv}) = \Delta_e$, which holds for any edge of M by the arbitrariness of the choice of the edge e_{uv}. Similar to the discussion of the graph energy of G, it can be obtained that

$$\mathcal{E}(G) = 2\sqrt{2\Delta_e + 1} + \mathcal{E}(G - e) = \cdots = 2k\sqrt{2\Delta_e + 1} + \mathcal{E}(G - ke).$$

Thus, $\mathcal{E}(G - ke) = 2(\mu(G) - k)\sqrt{2\Delta_e + 1}$. Since M is a maximum matching of G, then $\mu(G - ke) = \mu(G) - k$ Thus, $\mathcal{E}(G - ke) = 2\mu(G - ke)\sqrt{2\Delta_e + 1}$, If Δ_e is odd, the result can be proved similarly. ■

Let $G = G_1 \cup G_2 \cup \cdots \cup G_q$, where $G_i (1 \leq i \leq q)$ are the components of G.

Lemma 13. *Let G_i be a non-trivial component of G. If Δ_e is even, then G_i has a perfect matching.*

Proof. Let M_{G_i} be a maximum matching of G_i. Assume that G_i has no perfect matching, then there exists a vertex $x \in V(G_i)$ such that x is incident with no edge of M_{G_i}. Then $|V(G_i)| \geq 3$. Assume that y is adjacent to x and $e_{yz} \in M_{G_i}$, where e_{yz} denotes the edge with endpoints y and z. Let R be a connected graph obtained from G by removing all the edges of $M \setminus \{e_{yz}\}$ from G and together with their endpoints. Then $\mu(R) = 1$ and thus $R \cong C_3 = xyz$ or $R \cong S_k$, where $k \geq 3$ and $x, y, z \in V(S_k)$. If $R \cong C_3 = xyz$, $\Delta_e \geq 2$, by Lemma 12, we have

$$\mathcal{E}(C_3) = 2\mu(C_3)\sqrt{2\Delta_e + 1} = 2\sqrt{2\Delta_e + 1} \geq 2\sqrt{5},$$

which contradicts with the fact that $\mathcal{E}(C_3) = 4$. If $R \cong S_k$ $(k \geq 3)$, since $\Delta_e \geq k - 2$, then by Lemma 12, we have

$$\mathcal{E}(S_k) = 2\mu(S_k)\sqrt{2\Delta_e + 1} = 2\sqrt{2\Delta_e + 1} \geq 2\sqrt{2k - 3},$$

which contradicts with the fact that $\mathcal{E}(S_k) = 2\sqrt{k-1}$. Thus, if Δ_e is even, then G_i has a perfect matching. ■

As discussed in the proof of Lemma 13, for the graph G and its maximum matching M, let e_{yz} be an edge of M, and let R be a connected graph obtained from G by removing all the edges of $M \setminus \{e_{yz}\}$ from G and together with their endpoints.

Lemma 14. *If Δ_e is odd, then $R \cong P_3$.*

Proof. Since $\mu(R) = 1$, then $R \cong C_3$ or $R \cong S_k$, where $k \geq 2$. Note that $\sqrt{a + 2\sqrt{a}} + \sqrt{a - 2\sqrt{a}} \geq \sqrt{2a}$ with equality holds if and only if $a = 4$.

If $R \cong C_3$, then $\Delta_e \geq 3 > 2$ and $a = 2(\Delta_e + 1) \geq 8$. By Lemma 12, we have

$$\mathcal{E}(C_3) = \mu(C_3)\left(\sqrt{a + 2\sqrt{a}} + \sqrt{a - 2\sqrt{a}}\right) > \sqrt{2a} \geq 4,$$

which contradicts with the fact that $\mathcal{E}(C_3) = 4$.

If $R \cong S_2$, then $\Delta_e \geq 1$ and $a = 2(\Delta_e + 1) \geq 4$. By Lemma 12, we have

$$\mathcal{E}(S_2) = \mu(S_2)\left(\sqrt{a + 2\sqrt{a}} + \sqrt{a - 2\sqrt{a}}\right) \geq \sqrt{2a} \geq 2\sqrt{2},$$

which contradicts with $\mathcal{E}(S_2) = 2$.

If $R \cong S_k$ $(k \geq 4)$, then $\Delta_e \geq k-2$ and $a = 2(\Delta_e + 1) \geq 2(k-1) \geq 6$. By Lemma 12, it is obvious that

$$\mathcal{E}(S_k) = \mu(S_k)\left(\sqrt{a+2\sqrt{a}} + \sqrt{a-2\sqrt{a}}\right) > \sqrt{2a} \geq 2\sqrt{k-1},$$

which contradicts with the fact that $\mathcal{E}(S_k) = 2\sqrt{k-1}$. Therefore, if Δ_e is odd, then $R \cong P_3$. ■

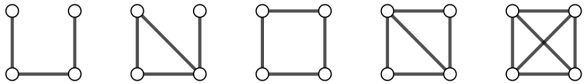

Figure 3. five possibilities for H_i.

Theorem 15. *Let G be an n-vertex graph with matching number $\mu(G)$ and maximum edge degree Δ_e.*

(i) *If Δ_e is even, then $\mathcal{E}(G) = 2\mu(G)\sqrt{2\Delta_e + 1}$ if and only if $G \cong \mu(G)P_2 \cup (n - 2\mu(G))K_1$.*

(ii) *If Δ_e is odd, then $\mathcal{E}(G) = \mu(G)(\sqrt{a+2\sqrt{a}} + \sqrt{a-2\sqrt{a}})$ with $a = 2(\Delta_e + 1)$ if and only if $G \cong \mu(G)P_3 \cup (n - 3\mu(G))K_1$.*

Proof. (i) Let G be a graph with $\mathcal{E}(G) = 2\mu(G)\sqrt{2\Delta_e + 1}$, where Δ_e is even. By Lemma 13, the order of each nontrivial connected component of G is even. Let G_i be a nontrivial component of G such that $G_i \ncong P_2$. Then $|V(G_i)| \geq 4$ and $\mu(G_i) \geq 2$. We confirm that G_i contains a connected induced subgraph H_i such that $\mu(H_i) = 2$. If $\mu(G_i) = 2$, then let $H_i = G_i$. If $\mu(G_i) > 2$, after deleting some edges in a maximum matching of G_i, we can construct a connected induced subgraph H_i of G_i such that $\mu(H_i) = 2$. Then H_i is isomorphic to P_4, $G(1,0,1)$, C_4, G_1 or K_4 as shown in Figure 3, where G_1 is a graph obtained from a cycle $u_1u_2u_3u_4$ by adding an edge u_1u_3. The energy of the graphs shown in Figure 3 are 4.47, 4.96, 4, 5.12 and 6, respectively. For each possibility, it is easy to verify that $\mathcal{E}(H_i) < 2\mu(H_i)\sqrt{2\Delta_e + 1}$, which contradicts with Lemma 12. Therefore, for an n-vertex graph G with Δ_e even, if $\mathcal{E}(G) = 2\mu(G)\sqrt{2\Delta_e + 1}$, then $G \cong \mu(G)P_2 \cup (n - 2\mu(G))K_1$.

If $G \cong \mu(G)P_2 \cup (n - 2\mu(G))K_1$, then $\Delta_e = 0$ and $\mathcal{E}(G) = 2\mu(G) = 2\mu(G)\sqrt{2\Delta_e + 1}$.

Thus, for an n-vertex graph G whose maximum edge degree Δ_e is even, $\mathcal{E}(G) = 2\mu(G)\sqrt{2\Delta_e+1}$ if and only if $G \cong \mu(G)P_2 \cup (n-2\mu(G))K_1$.

(ii) Let G be a graph with $\mathcal{E}(G) = \mu(G)(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}})$ where $a = 2(\Delta_e+1)$ and Δ_e is odd. Now let G_i is a connected component of G with $\mu(G_i) \geq 2$, and let G_i' is a connected subgraph of G_i with $\mu(G_i') = 2$ obtained by deleting some edges in a maximum matching in G_i. Then by Lemma 14, G_i' is C_5, $T(2,2)$, $G(1,1,1)$, $K_{2,3}$ or G_2 as shown in Figure 4, where G_2 is a graph obtained from a complete bipartite graph $K_{2,3}$ whose vertex set is $\{u_1,u_2,v_1,v_2,v_3\}$ by adding a new edge u_1u_2.

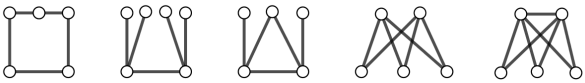

Figure 4. five possibilities for G_i'.

The energy of the graphs shown in Figure 4 are 6.47, 6, 5.84, 4.90 and 6, respectively. For each possibility, it is easy to verify that $\mathcal{E}(G_i') < \mu(G_i')\big(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}}\big)$, contradicting with Lemma 12. Then for each nontrivial connected component G_i of G, we have $\mu(G_i) = 1$. It follows from Lemma 14 that each nontrivial connected component of G is P_3. Therefore, for an n-vertex graph G with Δ_e odd, if $\mathcal{E}(G) = \mu(G)(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}})$ with $a = 2(\Delta_e+1)$, then $G \cong \mu(G)P_3 \cup (n-3\mu(G))K_1$.

If $G \cong \mu(G)P_3 \cup (n-3\mu(G))K_1$, then $\Delta_e = 1$, $a = 2(\Delta_e+1) = 4$ and $\mathcal{E}(G) = 2\sqrt{2}\mu(G) = \mu(G)(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}})$.

Thus, for an n-vertex graph G whose maximum edge degree Δ_e is odd, $\mathcal{E}(G) = \mu(G)(\sqrt{a+2\sqrt{a}}+\sqrt{a-2\sqrt{a}})$ with $a = 2(\Delta_e+1)$ if and only if $G \cong \mu(G)P_3 \cup (n-3\mu(G))K_1$. ■

Acknowledgments: This work was supported by the National Natural Science Foundation of China (Grant Nos. 11871206,61773020). The authors would like to express their sincere gratitude to all the referees for their careful reading and insightful suggestions.

References

[1] N. Alawiah, N. Rad, A. Jahanbani, H. Kamarulhaili, New upper bounds on the energy of a graph, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 287–301.

[2] F. Ashraf, On energy of trees with perfect matching, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 439–442.

[3] C. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, *Proc. Camb. Phil. Soc.* **36** (1940) 201–203.

[4] K. C. Das, S. Mojallal, Upper bounds for the energy of graphs, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 657–662.

[5] K. C. Das, I. Gutman, Bounds for graph energy, *Hacettepe J. Math. Stat.* **45** (2016) 695–703.

[6] J. Day, W. So, Graph energy change due to edge deletion, *Lin. Algebra Appl.* **428** (2008) 2070–2078.

[7] K. Fan, Maximum properties and inequalities for the eigenvalues of completely continuous operators, *Proc. Natl. Acad. Sci. USA.* **37** (1951) 760–766.

[8] C. Godsil, I. Gutman, On the theory of the matching polynomial, *J. Graph Theory* **5** (1981) 137–144.

[9] I. Gutman, The energy of a graph, *Ber. Math. Stat. Sekt. Forschungsz. Graz* **103** (1978) 1–22.

[10] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.

[11] Y. Hou, Z. Tang, C. Woo, On the spectral radius, k-degree and the upper bound of energy of a graph in a graph, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 341–350.

[12] J. Koolen, V. Moulton, Maximal energy graphs, *Adv. Appl. Math.* **26** (2001) 47–52.

[13] J. Koolen, V. Moulton, Maximal energy bipartite graphs, *Graphs Comb.* **19** (2003) 131–135.

[14] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.

[15] B. McClelland, Properties of the latent roots of a matrix: the estimation of π-electron energies, *J. Chem. Phys.* **54** (1971) 640–643.

[16] J. Rada, A. Tineo, Upper and lower bounds for the energy of bipartite graphs, *J. Math. Anal. Appl.* **289** (2004) 446–455.

[17] S. Renqian, Y. Ge, B. Huo, S. Ji, Q. Diao, On the tree with diameter 4 and maximum energy, *Appl. Math. Comput.* **268** (2015) 364–374.

[18] F. Tian, D. Wong, Upper bounds of the energy of triangle–free graphs in terms of matching number, *Lin. Multilin. Algebra.* **67** (2019) 20–28.

[19] D. Wong, X. Wang, R. Chu, Lower bounds of graph energy in terms of matching number, *Lin. Algebra Appl.* **549** (2018) 276–286.

[20] L. Wang, X. Ma, Bounds of graph energy in terms of vertex cover number, *Lin. Algebra Appl.* **517** (2017) 207–216.