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Energy Change of Graphs Due to Edge Addition

Huahui Ding, Danyi Li*, Weigen Yan*

School of Sciences, Jimei University, Xiamen 361021, China

2365430677@qq.com; danyilee1007@163.com; weigenyan@263.net

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Abstract

Let $G = (V(G), E(G))$ be a graph with adjacency matrix $A(G)$. The energy $\mathcal{E}(G)$ of G is defined as the sum of the absolute values of eigenvalues of $A(G)$. An open problem posed by Gutman is to determine how to change the energy of graphs when an edge is deleted or added. In this paper, we prove that, for a bipartite graph G and $e \in E(G^c)$, if each cycle C_i of $G + e$ containing e has length $|V(C_i)| \not\equiv 0$ $(mod\ 4)$, then $\mathcal{E}(G) < \mathcal{E}(G + e)$, where G^c is the complement of G. We also prove that, for a tree T and $e = uv \in E(T^c)$, if the unique cycle C of $T + e$ satisfies $|V(C)| \equiv 0$ $(mod\ 4)$ and there exists a pendent vertex of $T + e$ adjacent with one of vertices of C different from u and v, then $\mathcal{E}(T) < \mathcal{E}(T + e)$.

1 Introduction

Throughout this paper, we only consider simple graphs. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. Denote the adjacency matrix of G by $A(G)$. The characteristic polynomial of G, denoted by $\Phi(G, x)$, is defined

*Corresponding author.

as the characteristic polynomial of $A(G)$. That is,

$$\Phi(G,x) = \det(xI - A(G)) = \sum_{i=0}^{n} a_i(G)x^{n-i},$$

where I is an identity matrix of order n. Thus G and its adjacency matrix $A(G)$ have the same eigenvalues, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$. The set of eigenvalues of G is called its spectrum. Graph energy is an important graph spectral invariant [17] defined as the sum of the absolute values of its eigenvalues. That is,

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

The concept of graph energy was first introduced by Gutman [7] based on findings during his research in theoretical chemistry. He discovered that there was a correlation between the total π-electron energy in molecules of conjugated hydrocarbons and the energy of the molecular graphs in Hückel Molecular Orbital (HMO) theory [9, 11]. The graph energy has been the subject of extensive study and research in the fields of mathematics [8,9,11] and chemistry [10, 16].

An intriguing topic in the study of graph energy is how the graph energy changes [4, 5, 19] when the edge set of a graph changes. In 2001, Gutman [8] proposed to characterize the graphs G and their edges e for which $\mathcal{E}(G-e) < \mathcal{E}(G)$. This problem has been studied by many researchers. Day and So in [4, 5] utilized a classical inequality for singular values of a matrix sum to analyze graph energy changes due to edge deletions and proved that the graph energy decreases when a cut edge is deleted as follows.

Lemma 1 ([5]). *If e is a cut edge in a simple graph G, then $\mathcal{E}(G-e) < \mathcal{E}(G)$.*

Gutman and Shao [12] used the Ky Fan inequality to extend the discussion of Day and So in [4, 5] to the case of weighted graphs. Shan et al. [21] and Gutman et al. [12] studied some sufficient conditions for the energy change of the single-cycle or bipartite graph to decrease when a non-cut edge is deleted, where a graph is called single-cycle if it contains a unique cycle (Obviously, if a single-cycle graph is connected, then it is a unicyclic graph).

Lemma 2 ([12, 21]). *Let G be a single-cycle or bipartite graph, and e be a non-cut edge of G. Denote by $\mathcal{C}_e(G)$ the set of all cycles containing e in G. Suppose that each cycle C in $\mathcal{C}_e(G)$ satisfies $|V(C)| \not\equiv 0 \ (mod\ 4)$, then $\mathcal{E}(G-e) < \mathcal{E}(G)$.*

Cioăba [5] studied the family of graphs with energy increases when an edge is removed, and found the regular complete bipartite $K_{n,n}$ of order $2n$ with $n \geq 2$ has this property. That is, $\mathcal{E}(K_{n,n}) < \mathcal{E}(K_{n,n}-e)$ for any edge $e \in E(K_{n,n})$. Akbari, Ghorbani and Oboudi [1], and Shan, He and Yu [20] in turn extended to complete multipartite graphs: For any edge e of $K_{n_1,n_2,\ldots,n_k}$, if $k \geq 2, n_i \geq 2$ for $1 \leq i \leq k$, then $\mathcal{E}(K_{n_1,n_2,\ldots,n_k}) < \mathcal{E}(K_{n_1,n_2,\ldots,n_k}-e)$. And if $\min\{n_1, n_2, \ldots, n_k\} = 1$, how does the energy of $K_{n_1,n_2,\ldots,n_k}$ change when e is deleted.

Wang and So [23] stated that the cycle C_n with n vertices has more energy than the path P_n with n vertices except $n = 4$, that is, for a cycle graph C_n, if $n \neq 4$, then $\mathcal{E}(C_n - e) < \mathcal{E}(C_n)$. Shan et al. [21] and Zhu [26] presented several novel edge grafting operations, and examined their impact on the energy of unicyclic graphs and bipartite graphs. Recently, Tang et al. [22] gave a new sufficient condition for $\mathcal{E}(G-e) < \mathcal{E}(G)$ where e is not necessarily to be a cut edge.

Although there has been extensive research on the graph energy, the question of how edge modifications affect graph energy is still not completely solved. This property of energy change has been applied to study extremal energy problems on certain graph classes, and it has great research value [6, 9, 13–15, 18, 24, 25].

In this paper, we mainly consider that some sufficient conditions such that $\mathcal{E}(G) < \mathcal{E}(G+e)$ for a bipartite graph G, where $e \in E(G^c)$. These extend the problem posed by Gutman in [8]. We mainly prove the following Theorems 1 and 2.

Theorem 1. *Let G be a bipartite graph and $e \in E(G^c)$. If each cycle C_i of $G+e$ containing e has length $|V(C_i)| \not\equiv 0 \ (mod\ 4)$, then $\mathcal{E}(G) < \mathcal{E}(G+e)$.*

Theorem 2. *Let T be a tree and $e = uv \in E(T^c)$. If the unique cycle C of $T + e$ satisfies $|V(C)| \equiv 0 \pmod 4$ and there exists a pendent vertex w of $T + e$ adjacent with one of vertices of C different from u and v, then $\mathcal{E}(T) < \mathcal{E}(T + e)$.*

Remark 1. *Let G be a bipartite graph with bipartition (V_1, V_2) in Theorem 1. Then, for any edge $e = xy \in E(G^c)$ such that $x, y \in V_1$ or $x, y \in V_2$, $G+e$ is non-bipartite and each cycle C of $G+e$ containing e satisfies $|V(C)| \equiv 1$ or $3 \pmod 4$. Hence there exist many edges $e \in E(G^c)$ in a bipartite graph G satisfy the condition in Theorem 1. Particularly, Theorem 1 is different from the result in Lemma 2.*

Remark 2. *Note that Shan, Shao, Gong, et.al [21] and Gutman, Shao [12], proved that, for a tree T and $e \in E(T^c)$, if the unique cycle C of $T+e$ satisfies $|V(C)| \not\equiv 0 \pmod 4$, then $\mathcal{E}(T) < \mathcal{E}(T+e)$. A natural question is: If $|V(C)| \equiv 0 \pmod 4$, how about $\mathcal{E}(T)$ and $\mathcal{E}(T+e)$? Theorem 2 answers partially this question.*

In the next section, we first present some preliminaries. In Section 3, we give proofs of Theorems 1 and 2.

2 Preliminaries

In this section, we introduce a way of comparing the energies of two graphs $G+e$ and G. This method is based on the Coulson integral formula. Secondly, we introduce several lemmas that play a key role in proving the main results.

2.1 A technique for comparing the energies of $G + e$ and G

The well-known Coulson integral formula [8, 11, 16] shows that the energy $\mathcal{E}(G)$ of a graph G can also be expressed in terms of the coefficients of its characteristic polynomials $\Phi(G,x)$ as follows:

$$\mathcal{E}(G)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\log\left[\left(\sum_{j=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^j a_{2j}(G)x^{2j}\right)^2 + \left(\sum_{j=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^j a_{2j+1}(G)x^{2j+1}\right)^2\right]dx.$$

For any graphs G_1 and G_2 with n vertices, here we may define the quasi-order "$\preceq$", similar to the one in [11,16], as $G_1 \preceq G_2$ if

$$0 \le (-1)^j a_{2j}(G_1) \le (-1)^j a_{2j}(G_2)$$

and

$$0 \le (-1)^j a_{2j+1}(G_1) \le (-1)^j a_{2j+1}(G_2) \quad \text{or}$$
$$0 \le (-1)^{j+1} a_{2j+1}(G_1) \le (-1)^{j+1} a_{2j+1}(G_2)$$

for all j. Furthermore, if there is at least one index j in the above inequalities such that the inequality holds strictly, then we say $G_1 \prec G_2$. Obviously, the increase in graph energy is positively related to the quasi-order. In other words,

$$G_1 \preceq G_2 \Longrightarrow \mathcal{E}(G_1) \le \mathcal{E}(G_2),\ G_1 \prec G_2 \Longrightarrow \mathcal{E}(G_1) < \mathcal{E}(G_2).$$

2.2 Some Lemmas

For bipartite graphs, the coefficients of characteristic polynomials are related to the following lemma.

Lemma 3 ([2,3])**.** *Let G be a bipartite graph. Then $(-1)^j a_{2j}(G) \ge 0$ and $a_{2j+1}(G) = 0$ for all j. Particularly, if T is a tree or a forest, then $(-1)^j a_{2j}(T)$ equals the number of j-matchings of T.*

A j-matching of G is defined here as a subgraph of G consisting of j disjoint edges. Denote $m(G,j)$ by the number of j-matchings of G. In general, to study the characteristic polynomial of a graph, we typically pay attention to the following crucial lemma.

Lemma 4 ([3]). *The characteristic polynomial of graph G satisfies:*

$$\Phi(G,x) = \Phi(G-e,x) - \Phi(G-u-v,x) - 2\sum_{C_e \in \mathcal{C}_e(G)} \Phi(G-C_e,x),$$

where $\mathcal{C}_e(G)$ denotes the set of all cycles containing edge $e = uv$ in G, and the sum ranges over all cycles C_e in $\mathcal{C}_e(G)$.

3 Proofs of Theorems 1 and 2

Now, we can give the proofs of our main results as follows.

Proof of Theorem 1. Let G be a bipartite graph with $n = |V(G)| = |V_1 \cup V_2|$ vertices and bipartition (V_1, V_2). Let $e = uv \in E(G^c)$ and let $\mathcal{C}_e(G+e)$ be the set of all cycles containing $e = uv$ in $G+e$.

If there exists a cycle $C \in \mathcal{C}_e(G+e)$ such that $|V(C)|$ is even, then $u \in V_1, v \in V_2$ or $u \in V_2, v \in V_1$. Hence $G+e$ is bipartite. Note that each cycle C_i of $G+e$ containing e has length $|V(C_i)| \not\equiv 0 \ (mod\ 4)$. By Lemma 2, then $\mathcal{E}(G+e) > \mathcal{E}(G)$.

We assume that, for any cycle $C \in \mathcal{C}_e(G+e)$, $|V(C)| \equiv 1 \ (mod\ 2)$, i.e., $|V(C)| \equiv 1$ or $3 \ (mod\ 4)$. Obviously, $u, v \in V_1$ or $u, v \in V_2$. We first prove the following claim.

Claim. For any possible positive integer j,

$$0 \le (-1)^j a_{2j}(G) \le (-1)^j a_{2j}(G+e). \tag{1}$$

Particularly, $-a_2(G) = |E(G)| < |E(G+e)| = -a_2(G+e)$.

By Lemma 4,

$$\Phi(G+e,x) = \Phi(G,x) - \Phi(G-u-v,x) - 2\sum_{C \in \mathcal{C}_e(G+e)} \Phi(G-C,x).$$

Denote by n_c the number of vertices of C and $p = \min\{n_c | C \in \mathcal{C}_e(G+$

$e)\}$. Hence, if $2 \le s < p$, then

$$a_s(G+e) = a_s(G) - a_{s-2}(G-u-v),$$

if $s \ge p$, then

$$a_s(G+e) = a_s(G) - a_{s-2}(G-u-v) - 2 \sum_{C \in \mathcal{C}_e(G+e)} a_{s-n_c}(G-C).$$

Note that $G - C$ is bipartite for each $C \in \mathcal{C}_e(G+e)$, and both $n-1$ and $n - n_c = |V(G-C)|$ have the same parity. It is not difficult to show that, for any $0 \le j \le \lfloor \frac{n}{2} \rfloor$, $a_{2j-n_c}(G-C) = 0$ if $n_c \le 2j \le n$, that is,

$$a_{2j}(G+e) = a_{2j}(G) - a_{2j-2}(G-u-v). \tag{2}$$

Multiplying both sides of Eq. (2) by $(-1)^j$, we obtain

$$(-1)^j a_{2j}(G+e) - (-1)^j a_{2j}(G) = (-1)^{j-1} a_{2j-2}(G-u-v). \tag{3}$$

Note that both $G-u-v$ and G are bipartite graphs. By Lemma 3,

$$(-1)^{j-1} a_{2j-2}(G-u-v) \ge 0, (-1)^j a_{2j}(G) \ge 0.$$

Hence, by Eq. (3), the claim holds.

Using the well-known Coulson integral formula and the claim above,

$$\begin{aligned}\mathcal{E}(G+e) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \Bigg[\left(\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^j a_{2j}(G+e) x^{2j} \right)^2 \\ + \left(\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^j a_{2j+1}(G+e) x^{2j+1} \right)^2 \Bigg] dx \\ \ge \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left(\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^j a_{2j}(G+e) x^{2j} \right)^2 dx\end{aligned}$$

$$> \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\log\left(\sum_{j=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^j a_{2j}(G)x^{2j}\right)^2 dx$$
$$= \mathcal{E}(G)$$

which implies that the theorem holds.

Proof of Theorem 2. Note that the unicyclic graph $T+e$ with the unique cycle C of length $l \equiv 0$ $(mod\ 4)$. Hence both T and $T+e$ are bipartite graphs. By Lemma 3, $a_{2j+1}(T) = a_{2j+1}(T+e) = 0$, $(-1)^j a_{2j}(T) \geq 0$ and $(-1)^j a_{2j}(T+e) \geq 0$.

For convenience, set $b_s(T) = (-1)^s a_{2s}(T)$ and $e = uv$. Then

$$\Phi(T,x) = \sum_{s=0}^{\lfloor n/2\rfloor}(-1)^s b_s(T)x^{n-2s},\ \ \Phi(T+e,x) = \sum_{s=0}^{\lfloor n/2\rfloor}(-1)^s b_s(T+e)x^{n-2s}.$$

Since $b_1(T+e) = |E(T+e)| > |E(T)| = b_1(T)$, by the Coulson integral formula, to prove $\mathcal{E}(T) < \mathcal{E}(T+e)$, it suffices to show that, for all $0 \leq j \leq \lfloor n/2\rfloor$,

$$b_j(T) \leq b_j(T+e).$$

By Lemma 4,

$$\Phi(T+e,x) = \Phi(T,x) - \Phi(T-u-v,x) - 2\Phi(T+e-C,x),$$

$$b_j(T+e) - b_j(T) = \begin{cases} b_{j-1}(T-u-v) \geq 0, & \text{if } j < l/2,\\ b_{j-1}(T-u-v) - 2b_{j-l/2}(T+e-C), & \text{otherwise.}\end{cases}$$

Note that $T-u-v$ and $T+e-C$ are forests which contain no cycle. Hence, for any $l/2 \leq j \leq \lfloor n/2\rfloor$, by Lemma 3,

$$b_{j-1}(T-u-v) = m(T-u-v, j-1),\ b_{j-l/2}(T+e-C) = m(T+e-C, j-l/2).$$

Let G_1 be the subgraph of $T+e$ induced by $\{w\}\cup V(C)\setminus\{u,v\}$, which is a path with $l-1$ vertices or a graph with $l-1$ vertices obtained from a path P_{l-2} with $l-2$ vertices by attaching a pendent edge to one of vertices of degree two in P_{l-2}. Obviously, $m(G_1, l/2-1) \geq 2$. Particularly,

$$\begin{aligned} m\left(T-u-v, j-1\right) &\geq m(G_1, l/2-1) \times m\left(T+e-C-w, j-l/2\right) \\ &= m(G_1, l/2-1) \times m\left(T+e-C, j-l/2\right) \\ &\geq 2m\left(T+e-C, j-l/2\right). \end{aligned}$$

So we have proved that, for all $0 \leq j \leq \lfloor n/2 \rfloor$, $b_j(T+e) \geq b_j(T)$. Hence the theorem follows.

References

[1] S. Akbari, E. Ghorbani, M. R. Oboudi, Edge addition, singular values, and energy of graphs and matrices, *Lin. Algebra Appl.* **430** (2009) 2192–2199.

[2] N. Biggs, *Algebraic Graph Theory*, Cambridge Univ. Press, New York, 1993.

[3] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.

[4] J. Day, W. So, Singular value inequality and graph energy change, *El. J. Lin. Algebra* **16** (2007) 291–299.

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

[6] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

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

[8] I. Gutman, The energy of a graph: old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann(Eds), *Algebraic Combinatorics and Applications*, Springer-Verlag, Berlin, 2001, pp. 196-211.

[9] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total π-electron energy on molecular topology, *J. Serb. Chem. Soc.* **70** (2005) 441–456.

[10] I. Gutman, M. Milun, N. Trinajstić, Huckel molecular orbital calculations of aromatic stabilization of annulenes, *Croat. Chem. Acta* **44** (1972) 207–213.

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

[12] I. Gutman, J. Y. Shao, The energy change of weighted graphs, *Lin. Algebra Appl.* **435** (2011) 2425–2431.

[13] Y. Hou, Unicyclic graphs with minimal energy, *J. Math. Chem.* **29** (2001) 163–168.

[14] F. Li, B. Zhou, Minimal energy of unicyclic graphs of a given diameter, *J. Math. Chem.* **43** (2008) 476–484.

[15] H. Li, On minimal energy ordering of acyclic conjugated molecules, *J. Math. Chem.* **25** (1999) 145–169.

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

[17] I. Milovanović, E. Milovanović, S. B. B. Altindağ , M. Matejić, McClelland-type upper bounds for graph energy, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 141–155.

[18] J. Rada, Energy ordering of catacondensed hexagonal systems, *Discr. Appl. Math.* **145** (2005) 437–443.

[19] O. Rojo, Effects on the energy and Estrada indices by adding edges among pendent vertices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 343–358.

[20] H. Y. Shan, C. X. He, Z. S. Yu, The energy change of the complete multipartite graph, *El. J. Lin. Algebra* **36** (2020) 309–317.

[21] H. Y. Shan, J. Y. Shao, F. Gong, Y. Liu, An edge grafting theorem on the energy of unicyclic and bipartite graphs, *Lin. Algebra Appl.* **433** (2010) 547–556.

[22] L. Tang, M. Lin, Q. Li, Graph energy change on edge deletion, *MATCH Commun. Math. Comput. Chem.* **90** (2023) 709–716.

[23] W. H. Wang, W. So, Graph energy change due to any single edge deletion, *El. J. Lin. Algebra* **29** (2015) 59–73.

[24] W. Yan, L. Ye, On the minimal energy of trees with a given diameter, *Appl. Math. Lett.* **18** (2005) 1046–1052.

[25] F. Zhang, Z. Li, L. Wang, Hexagonal chains with minimal total π-electron energy, *Chem. Phys. Lett.* **337** (2001) 125–130.

[26] J. Zhu, Two new edge grafting operations on the energy of unicyclic graphs and their applications, *Discr. Math.* **312** (2012) 3117–3127.