

The Energy Change of Graphs under Some Edges Deletions

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(Received March 17, 2025)

Abstract

The energy $\mathcal{E}(G)$ of a graph G is the sum of the absolute values of all the eigenvalues of its adjacency matrix. Gutman (2001) pointed out a problem to characterize the graph G and the edge e of G such that $\mathcal{E}(G - e) \leq \mathcal{E}(G)$. Tang et al. (2023) gave a sufficient condition for $\mathcal{E}(G - e) \leq \mathcal{E}(G)$, where e is not necessarily a cut-edge set or a cut edge. We deduce here a stronger conclusion than the results obtained by Tang et al. (2023). Our findings cover some known conclusions, such as the results obtained by Gutman and Pavlović (1999) and Tang et al. (2023). In addition, based on the new results we obtained in this article, we can directly conclude that adding edges to a complete k -partite graph leads to a graph with a higher energy than the energy of the original graph.

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1 Introduction

Let $G = (V(G), E(G))$ be a simple graph with n vertices, where $V(G) = \{v_1, v_2, \dots, v_n\}$ and $E(G)$ are the vertex set and edge set of G , respectively. Let $\mathbf{A}(G) = (a_{i,j})_{n \times n}$ denote the adjacency matrix of G with $a_{i,j} = 1$ if v_i is adjacent to v_j and $a_{i,j} = 0$ otherwise. Since $\mathbf{A}(G)$ is a real symmetric matrix, every eigenvalue of $\mathbf{A}(G)$ is real. Let $\lambda_i(G)$ denote the i -th largest eigenvalue of $\mathbf{A}(G)$, where $1 \leq i \leq n$. Namely, we have $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$. It is well known that $\lambda_1(G)$ is referred to as the spectral radius of the graph G . The energy of a graph G is defined as the sum of the absolute values of all the eigenvalues of $\mathbf{A}(G)$ [8]. We have

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

Graph energy is an important graph spectral invariant [13]. In theoretical chemistry, researchers have studied the energy of a graph extensively because it is connected to the total π -electron energy of the molecule that the graph represents. The graph energy helps people understand the chemical properties of the molecule through its graph structure [5, 7]. In studying the graph energy, one important area is focused on understanding how the energy of a graph alters when a subgraph is removed. In a survey paper [9] on the subject of graph energy, Gutman pointed out a “hard-to-crack” issue, as shown in Problem 1.

Problem 1. [9] *Characterize the graph G and their edges e such that $\mathcal{E}(G - e) \leq \mathcal{E}(G)$.*

Problem 1 and the related issues are called the graph energy change problem and they attracted many attentions among the community [2, 3, 8]. Day and So [2] studied graph energy changes due to edge deletions by using a classical inequality for the singular values of a matrix sum and they got $\mathcal{E}(G - e) \leq \mathcal{E}(G)$, where e is a cut edge. Wang and So [16] utilized three different ways to prove $\mathcal{E}(C_n - e) < \mathcal{E}(P_n)$, where C_n and P_n are respectively cycle graph and path graph with n vertices and $n \neq 4$. Li and So [11] constructed an infinite family of connected graphs

equienergetic with subgraphs of one edge fewer. Gutman and Shao [7] studied the condition for $\mathcal{E}(G - e) < \mathcal{E}(G)$, where G is a weighted graph. Ding et al. [4] considered some sufficient conditions such that $\mathcal{E}(G) < \mathcal{E}(G + e)$ for a bipartite graph G , where $e \in E(G^c)$ and G^c is a complement of G .

Gutman and Pavlović [6] studied the graph energy change and they introduced the definition of the graph $Kc_n(k)$ as follows.

Definition 1. [6] Let W_k be a k -element subset of the vertex set of the complete graph K_n , where $2 \leq k \leq n$ and $n \geq 3$. The graph $Kc_n(k)$ is obtained by deleting, from K_n , all the edges connecting pairs of vertices in W_k . In addition, $Kc_n(0) \equiv Kc_n(1) \equiv K_n$.

By using the characteristics polynomial of graphs and the spectral methods, Gutman and Pavlović [6] obtained the following Theorem 1.

Theorem 1. [6] $\mathcal{E}(Kc_n(k)) < \mathcal{E}(K_n)$, where $2 \leq k \leq n$ and $n \geq 3$.

For $Kc_n(k)$, if $k = 2$, then $Kc_n(2)$ is derived from the complete graph K_n by deleting an edge. By Theorem 1, we get $\mathcal{E}(K_n - e) < \mathcal{E}(K_n)$ for any edge e of K_n .

The following observation of Cioăba [2] provides an infinite family of graphs with the property of energy increased.

Theorem 2. [2] If $K_{n,n}$ is the regular complete bipartite graph of order $2n$ with $n \geq 2$, then $\mathcal{E}(K_{n,n}) < \mathcal{E}(K_{n,n} - e)$ for any edge e of $K_{n,n}$.

A complete k -partite graph, denoted by K_{t_1, \dots, t_k} , is a graph whose vertices can be divided into k disjoint sets in such a way that no two vertices within the same set are adjacent and every pair of vertices in K_{t_1, \dots, t_k} from different sets is adjacent, where $k \geq 2$ and $t_i \geq 1$ for $1 \leq i \leq k$. Akbari et al. [1] avoided the hard calculation of eigenvalues and generalized the results of Theorem 2 to Theorem 3.

Theorem 3. [1] $\mathcal{E}(K_{t_1, \dots, t_k}) < \mathcal{E}(K_{t_1, \dots, t_k} - e)$ for any edge e of K_{t_1, \dots, t_k} , where $k \geq 2$ and $t_i \geq 2$ for $1 \leq i \leq k$.

Later, Shan et al. [14] introduced a new method to study the graph energy and they completely determined how the energy of K_{t_1, \dots, t_k} changes when one edge is deleted for $\min\{t_1, \dots, t_k\} = 1$.

For a graph G and a vertex u in $V(G)$, let $N_G(u)$ be the set of neighbors of u . Without confusion, we use $N(u)$ instead of $N_G(u)$. For a subset V' of $V(G)$, let $G[V']$ represent the induced subgraph of G . Namely, the vertex set of $G[V']$ is V' and $G[V']$ contains all the edges that have both endpoints in V' .

Recently, Tang et al. [15] obtained Theorem 4 as follows.

Theorem 4. [15] *Suppose that G is a graph of order n with a given vertex set U such that the induced subgraph $G[U]$ is a regular complete bipartite graph $K_{a,a}$, and $N(v) \setminus U = N(u) \setminus U$ for any $v, u \in U$. Then $\mathcal{E}(G) > \mathcal{E}(G - E(G[U]))$, i.e., deleting all the edges of $G[U]$ from G will decrease $\mathcal{E}(G)$.*

The property of energy change is of practical importance for researchers to investigate the extremal energy problems among some graph classes. Although researchers have obtained some relevant conclusions for Problem 1, Problem 1 is still far from being completely resolved.

In this article, we further study the sufficient conditions for $\mathcal{E}(G) > \mathcal{E}(G - E')$ and $\mathcal{E}(G) < \mathcal{E}(G + E')$, where G is a graph of order n and E' is an edge set. The main results of this article are shown in Theorems 5–7 and Corollary 1 in Section 2. In Theorem 5, we release the conditions of Theorem 4 and obtain a stronger conclusion than Theorem 4. Then by Theorem 5, we get Theorems 6 and 7. Theorem 6 covers some known results, such as Theorem 1 obtained by Gutman and Pavlović [6] and Lemma 1 in [15] (as shown in Corollary 1). Theorem 7 yields some new results.

2 Main results

In this section, we obtain the main results of this article. To obtain our results, we first introduce Lemmas 1–3. Lemma 1 is a useful lemma for us to compare the spectral radii of two graphs. Lemma 2 gives us a sufficient condition to compare the energies of two graphs.

Lemma 1. [12] *Let G be a connected graph, and let G' be a proper spanning subgraph of G . Then $\rho(G) > \rho(G')$.*

Lemma 2. Let G_1 and G_2 be two n -vertex graphs with the same vertex set, where $n \geq 3$. We assume that $\lambda_{k+1}(G_1)$ ($1 \leq k \leq n-1$) is the first eigenvalue of $\mathbf{A}(G_1)$ which is equal to or smaller than zero, i.e., $\lambda_i(G_1) > 0$ for $1 \leq i \leq k$ and $\lambda_i(G_1) \leq 0$ for $k+1 \leq i \leq n$. If $\lambda_1(G_2) > \lambda_1(G_1)$ and $\lambda_i(G_2) \geq \lambda_i(G_1)$ for $2 \leq i \leq k$, then we have $\mathcal{E}(G_2) > \mathcal{E}(G_1)$.

Proof. Since $\lambda_k(G_1) > 0$, by the condition of Lemma 2, we obtain $\lambda_k(G_2) > 0$. If $\lambda_{k+1}(G_2) \leq 0$, we have $\mathcal{E}(G_2) = 2 \sum_{i=1}^k \lambda_i(G_2) > 2 \sum_{i=1}^k \lambda_i(G_1) = \mathcal{E}(G_1)$, where the inequality holds since $\lambda_1(G_2) > \lambda_1(G_1)$. If $\lambda_{k+1}(G_2) > 0$, we have $\mathcal{E}(G_2) > 2 \sum_{i=1}^k \lambda_i(G_2) > 2 \sum_{i=1}^k \lambda_i(G_1) = \mathcal{E}(G_1)$. \blacksquare

Let $\mathbf{x}_1, \dots, \mathbf{x}_n$ be n vectors, and $\text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ be the vector space spanned by those vectors.

Lemma 3. Let the $n \times n$ adjacency matrix \mathbf{A} of a simple undirected graph G of the form

$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{Y} \\ \mathbf{Y}^T & \mathbf{Z} \end{pmatrix},$$

where $\mathbf{0}$ is an $m \times m$ matrix with $1 \leq m \leq n-1$, $\mathbf{Y} = \mathbf{e}\mathbf{y}^T$ with \mathbf{e} being the all-1 vector and \mathbf{y} being a fixed $(0, 1)$ -vector.

(i) If $\mathbf{p} = \begin{pmatrix} \mathbf{p}' \\ \mathbf{p}'' \end{pmatrix}$ is an eigenvector of \mathbf{A} with respect to the nonzero eigenvalue λ , then $\mathbf{p}' = \alpha\mathbf{e}$ for some α .

(ii) If $\mathbf{x} = \begin{pmatrix} \mathbf{x}' \\ \mathbf{x}'' \end{pmatrix} \in \text{span}\{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_i\}$, where \mathbf{p}_t 's are eigenvectors of \mathbf{A} with respect to nonzero eigenvalues $\lambda_t(\mathbf{G})$ for $1 \leq t \leq i$, then $\mathbf{x}' = \mu\mathbf{e}$ for some μ .

(iii) Let $\mathbf{W} = \begin{pmatrix} \mathbf{X} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$ and $\mathbf{x} = \begin{pmatrix} \mathbf{x}' \\ \mathbf{x}'' \end{pmatrix}$ as in part (ii), where \mathbf{X} is a $(0, 1)$ -matrix with non-negative entries. Then $\mathbf{x}^T \mathbf{W} \mathbf{x} \geq 0$.

Proof. (i) By the definition of eigen-equation, we have

$$\begin{pmatrix} \mathbf{Y}\mathbf{p}'' \\ \mathbf{Y}^T\mathbf{p}' + \mathbf{Z}\mathbf{p}'' \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{Y} \\ \mathbf{Y}^T & \mathbf{Z} \end{pmatrix} \begin{pmatrix} \mathbf{p}' \\ \mathbf{p}'' \end{pmatrix} = \mathbf{A}\mathbf{p} = \lambda\mathbf{p} = \begin{pmatrix} \lambda\mathbf{p}' \\ \lambda\mathbf{p}'' \end{pmatrix}.$$

Hence $\mathbf{Y}\mathbf{p}'' = \lambda\mathbf{p}'$ and so $\mathbf{p}' = \frac{1}{\lambda}\mathbf{Y}\mathbf{p}'' = \frac{1}{\lambda}\mathbf{e}\mathbf{y}^T\mathbf{p}'' = \alpha\mathbf{e}$ with $\alpha = \frac{\mathbf{y}^T\mathbf{p}''}{\lambda}$.

(ii) This is clearly a result of part (i).

(iii) From part (ii), since \mathbf{X} is a $(0, 1)$ -matrix, we have $\mathbf{x}^T \mathbf{W} \mathbf{x} = (\mathbf{x}')^T \mathbf{X} \mathbf{x}' = (\mu \mathbf{e})^T \mathbf{X} (\mu \mathbf{e}) = \mu^2 (\mathbf{e}^T \mathbf{X} \mathbf{e}) \geq 0$. ■

Based on Theorem 4, we remove a constraint of Theorem 4 (namely, the induced subgraph $G[U]$ is a regular complete bipartite graph $K_{a,a}$) and obtain Theorem 5 as follows.

Theorem 5. *Let G be a graph of order n and V_0 be a given subset of $V(G)$, where $N(v) \setminus V_0 = N(u) \setminus V_0$ for any two vertices $v, u \in V_0$. If $E(G[V_0]) \neq \emptyset$, then $\mathcal{E}(G) > \mathcal{E}(G - E(G[V_0]))$.*

Proof. If G is not connected, we only need to consider the component containing all the vertices in V_0 since the energy of a graph equals to the sum of the energies of all its components. Let $G' = G - E(G[V_0])$ for simplicity. Next, we assume that G is connected. To obtain Theorem 5, we prove Claims 1 and 2 as follows.

Claim 1. $\lambda_1(G) > \lambda_1(G')$.

Proof. It is noted that G' is a proper subgraph of G since $E(G[V_0]) \neq \emptyset$. We have $\lambda_1(G) > \lambda_1(G')$ by Lemma 1. ■

We assume that $\lambda_{k+1}(G')$ is the first eigenvalue of $\mathbf{A}(G')$ which is equal to or smaller than zero, where $1 \leq k \leq n - 1$.

Claim 2. $\lambda_i(G) \geq \lambda_i(G') > 0$ for $2 \leq i \leq k$.

Proof. By the definition of $\lambda_{k+1}(G')$, we have $\lambda_i(G') > 0$ for $2 \leq i \leq k$. Next, we prove $\lambda_i(G) \geq \lambda_i(G') > 0$ for $2 \leq i \leq k$. Let $V(G) = \{v_1, v_2, \dots, v_n\}$ and $V_0 = \{v_1, v_2, \dots, v_m\}$, where $n \geq 3$ and $2 \leq m \leq n - 1$. It is noted that if $m = n$, then Theorem 5 obviously holds. For an arbitrary vertex v_i in V_0 , we have $|N(v_i) \setminus V_0| \geq 1$ since G is connected and $n > m$, where $1 \leq i \leq m$. Let $|N(v_i) \setminus V_0| = d$, where $1 \leq i \leq m$. Let $\mathbf{X} = \mathbf{A}(G[V_0])$, where \mathbf{X} is an $m \times m$ real symmetric matrix. Let $\mathbf{Z} = \mathbf{A}(G[V(G) - V_0])$. We assume $\mathbf{Y} = \begin{pmatrix} \mathbf{J}_{m \times d} & \mathbf{0}_{m \times (n-m-d)} \\ \mathbf{Y}^T & \mathbf{Z} \end{pmatrix}$, where $\mathbf{J}_{m \times d}$ is an $m \times d$ matrix whose entries are all 1. We have

$$\mathbf{A}(G) = \begin{pmatrix} \mathbf{X} & \mathbf{Y} \\ \mathbf{Y}^T & \mathbf{Z} \end{pmatrix}, \quad \mathbf{A}(G') = \begin{pmatrix} \mathbf{0}_{m \times m} & \mathbf{Y} \\ \mathbf{Y}^T & \mathbf{Z} \end{pmatrix}.$$

Let $\{\mathbf{p}_j\}_{j=1}^n$ and $\{\mathbf{q}_j\}_{j=1}^n$ be orthonormal lists of eigenvectors of $\mathbf{A}(G')$

and $\mathbf{A}(G)$ respectively. It is noted that the sequences $\{\mathbf{p}_j\}_{j=1}^n$ and $\{\mathbf{q}_j\}_{j=1}^n$ are organized such that their elements correspond to their eigenvalues in the same order. Let $\mathcal{S}_1 = \text{span}\{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_i\}$ and $\mathcal{S}_2 = \text{span}\{\mathbf{q}_i, \mathbf{q}_{i+1}, \dots, \mathbf{q}_n\}$, where i is fixed, $2 \leq i \leq k$, and $2 \leq k \leq n-1$. It is easy to check that $\dim(\mathcal{S}_1) = i$ and $\dim(\mathcal{S}_2) = n-i+1$. So there is a unit vector $\mathbf{x} \in \mathcal{S}_1 \cap \mathcal{S}_2$ since $i + (n-i+1) = n+1 > n$. Let $\mathbf{W} = \mathbf{A}(G) - \mathbf{A}(G')$. For $2 \leq i \leq k$ and $2 \leq k \leq n-1$, by the Rayleigh Theorem [10], we have

$$\begin{aligned}\lambda_i(G) &= \mathbf{q}_i^T \mathbf{A}(G) \mathbf{q}_i \geq \mathbf{x}^T \mathbf{A}(G) \mathbf{x} \\ &= \mathbf{x}^T \mathbf{A}(G') \mathbf{x} + \mathbf{x}^T \mathbf{W} \mathbf{x} \\ &\geq \mathbf{p}_i^T \mathbf{A}(G') \mathbf{p}_i + \mathbf{x}^T \mathbf{W} \mathbf{x} = \lambda_i(G') + \mathbf{x}^T \mathbf{W} \mathbf{x}.\end{aligned}\quad (2)$$

Since G' is a simple undirected graph with the adjacency matrix $\mathbf{A}(G') = \begin{pmatrix} \mathbf{0}_{m \times m} & \mathbf{Y} \\ \mathbf{Y}^T & \mathbf{Z} \end{pmatrix}$, where $\mathbf{Y} = \begin{pmatrix} \mathbf{J}_{m \times d} & \mathbf{0}_{m \times (n-m-d)} \end{pmatrix} = \mathbf{e} \mathbf{y}^T$ with \mathbf{e} being the all-1 vector and \mathbf{y} being a fixed $(0,1)$ -vector, we can directly get $\mathbf{x}^T \mathbf{W} \mathbf{x} \geq 0$ by Lemma 3. Thus, we have $\lambda_i(G) \geq \lambda_i(G')$ for $2 \leq i \leq k$ and $2 \leq k \leq n-1$.

By the combination of Lemma 2 and Claims 1 and 2, we have $\mathcal{E}(G) > \mathcal{E}(G - E(G[V_0]))$. ■

Remark: In Theorem 5, it does not require $G[V_0]$ to be a regular complete bipartite graph $K_{a,a}$. Since Theorem 5 only needs $N(v) \setminus V_0 = N(u) \setminus V_0$ for any two vertices $v, u \in V_0$, Theorem 5 can be applicable to a wider range of graphs than Theorem 4.

By using Theorem 5, we obtain Theorems 6 and 7 as follows.

Theorem 6. Let $U = \{U_1, U_2, \dots, U_p\}$ and $V = \{V_1, V_2, \dots, V_q\}$ be two sets, where $q > p \geq 0$, $U_i \subseteq V(K_n)$ for $1 \leq i \leq p$, $V_j \subseteq V(K_n)$ for $1 \leq j \leq q$, $|U_i| = |V_i|$ for $1 \leq i \leq p$, $U_i \cap U_j = \emptyset$ for $1 \leq i < j \leq p$, and $V_i \cap V_j = \emptyset$ for $1 \leq i < j \leq q$. We have $\mathcal{E}(K_n - \sum_{i=1}^p E(K_n[U_i])) > \mathcal{E}(K_n - \sum_{i=1}^q E(K_n[V_i]))$.

Proof. By the methods similar to those for the proofs of Lemma 1 in [15], we can obtain that $K_n - \sum_{i=1}^p E(K_n[U_i])$ is isomorphic to $K_n - \sum_{i=1}^p E(K_n[V_i])$.

Therefore, we have $\mathcal{E}(K_n - \sum_{i=1}^p E(K_n[U_i])) = \mathcal{E}(K_n - \sum_{i=1}^p E(K_n[V_i]))$. Furthermore, by using Theorem 5 $q-p$ times, we get $\mathcal{E}(K_n - \sum_{i=1}^p E(K_n[V_i])) > \mathcal{E}(K_n - \sum_{i=1}^q E(K_n[V_i]))$. Thus, Theorem 6 holds. ■

Remark: Theorem 6 covers some known results. For example, Theorem 1 obtained by Gutman and Pavlović [6] is a corollary of Theorem 6. In addition, by Theorem 6, we can easily get Corollary 1 as follows. It is noted that Corollary 1 is Lemma 1 in [15].

For completeness, we give the simple proofs of Theorem 1 and Corollary 1 as follows.

The new proof of Theorem 1. In Theorem 6, let $U = \emptyset$ and V_1 be W_k which is shown in Definition 1, where $k \geq 2$. Namely $p = 0$ and $q = 1$ in Theorem 6. By Theorem 6, we can directly get Theorem 1. ■

Corollary 1. Suppose that M_1 and M_2 are two matchings of K_n with $n \geq 2$. If $|M_1| < |M_2|$, then $\mathcal{E}(K_n - M_1) > \mathcal{E}(K_n - M_2)$.

Proof. In Theorem 6, if U and V are two matchings of K_n , namely $|U_i| = 2$ for $1 \leq i \leq p$ and $|V_j| = 2$ for $1 \leq j \leq q$, then Theorem 6 is Corollary 1. ■

For two given graphs G_1 and G_2 , the joint product of G_1 and G_2 , denoted by $G_1 + G_2$, is obtained from G_1 and G_2 by adding every possible edge between the vertices in G_1 and the vertices in G_2 .

Theorem 7. Let $k \geq 2$ and $t_i \geq 1$ for $1 \leq i \leq k$. We have $\mathcal{E}(K_{t_1, \dots, t_k}) < \mathcal{E}(G_{t_1} + G_{t_2} + \dots + G_{t_k})$, where G_{t_i} is an arbitrary simple graph having t_i vertices with $1 \leq i \leq k$ and there exists at least one i with $1 \leq i \leq k$ such that $|E(G_{t_i})| \geq 1$.

Proof. By using Theorem 5 at most k times, we can get Theorem 7. ■

Remark: In Theorem 7, since G_{t_i} is an arbitrary simple graph having t_i vertices, where $t_i \geq 1$ for $1 \leq i \leq k$ with $k \geq 2$, we know that $G_{t_1} + G_{t_2} + \dots + G_{t_k}$ is a graph obtained by adding edges to a complete k -partite graph K_{t_1, \dots, t_k} if there exists at least one i such that $|E(G_{t_i})| \geq 1$. Theorem 3 obtained by Akbari et al. [1] shows that if we delete an arbitrary edge e from K_{t_1, \dots, t_k} , then $\mathcal{E}(K_{t_1, \dots, t_k}) < \mathcal{E}(K_{t_1, \dots, t_k} - e)$ holds, where $t_i \geq 2$ for

$1 \leq i \leq k$ and $k \geq 2$. Naturally, it is interesting to ask how the energy changes if we add an edge to K_{t_1, \dots, t_k} . By Theorem 7, we can directly obtain that $\mathcal{E}(K_{t_1, \dots, t_k} + e) > \mathcal{E}(K_{t_1, \dots, t_k})$, where e is an edge, $t_i \geq 2$ for $1 \leq i \leq k$ and $k \geq 2$.

Acknowledgment: The work was supported by the Natural Science Foundation of Shanghai under the grant number 21ZR1423500.

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