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An edge grafting theorem on the energy of unicyclic and bipartite graphs ☆

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The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. The edge grafting operation on a graph is certain kind of edge moving between two pendant paths starting from the same vertex. In this paper we show how the graph energy changes under the edge grafting operations on unicyclic and bipartite graphs. We also give some applications of this result on the comparison of graph energies between unicyclic or bipartite graphs.

1. Introduction

Let G be a simple graph with n vertices and A be its adjacency matrix. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A, then the *energy* of G, denoted by $E(G)$, is defined [2,3] as $E(G) = \sum_{i=1}^{n} |\lambda_i|$.

In theoretical chemistry, the energy of a given molecular graph is related to the total π-electron energy of the molecule represented by that graph. So the graph energy has some specific chemical interests and has been extensively studied [2–4].

The characteristic polynomial $\det(xI - A)$ of the adjacency matrix A of a graph G is also called the characteristic polynomial of G, written as $\phi(G, x) = \sum_{i=0}^{n} a_i(G)x^{n-i}$. Using these coefficients of

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$\phi(G,x)$, the energy $E(G)$ of a graph G with n vertices can be expressed by the following Coulson integral formula [4]:

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\ln\left[\left(\sum_{j=0}^{\lfloor n/2\rfloor}(-1)^j a_{2j}(G)x^{2j}\right)^2 + \left(\sum_{j=0}^{\lfloor n/2\rfloor}(-1)^j a_{2j+1}(G)x^{2j+1}\right)^2\right]dx. \quad (1.1)$$

A unicyclic graph is a connected graph in which the number of edges equals the number of vertices. Obviously, a unicyclic graph contains a unique cycle. Conversely, if a graph contains a unique cycle, then it must be a disjoint union of a unicyclic graph and several trees. We call such graph as a *single-cycle* graph.

In this paper, we use $G(n,l)$ to denote the set of unicyclic graphs of order n whose unique cycle has length l, and use $G_1(n,l)$ to denote the set of single-cycle graphs of order n whose unique cycle has length l.

A graph G is called a UOB graph, if it is a unicyclic graph or a bipartite graph.

Throughout this paper, we write:

$$b_i(G) = |a_i(G)|, \qquad \text{where } \phi(G,x) = \sum_{i=0}^{n} a_i(G)x^{n-i}.$$

It is easy to see that $b_0(G) = 1$, $b_1(G) = 0$, and $b_2(G)$ equals the number of edges of G.

The following results related to the signs of the coefficients of the characteristic polynomials are both true for single-cycle graphs [5] and bipartite graphs [1].

Lemma 1.1. *Let G be a single-cycle graph or a bipartite graph. Then:*

(1) $b_{2j}(G) = (-1)^j a_{2j}(G)$.
(2) $b_{2j+1}(G) = (-1)^j a_{2j+1}(G)$, *if G contains a cycle of length l with* $l \not\equiv 1 (mod\ 4)$.
(3) $b_{2j+1}(G) = (-1)^{j+1} a_{2j+1}(G)$, *if G contains a cycle of length l with* $l \equiv 1 (mod\ 4)$.

From Lemma 1.1, the Coulson integral formula (1.1) can be rewritten as the following form (in terms of $b_i(G)$) for UOB graphs:

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\ln\left[\left(\sum_{j=0}^{\lfloor n/2\rfloor} b_{2j}(G)x^{2j}\right)^2 + \left(\sum_{j=0}^{\lfloor n/2\rfloor} b_{2j+1}(G)x^{2j+1}\right)^2\right]dx. \quad (1.2)$$

It follows that $E(G)$ is a strictly monotonically increasing function of those numbers $b_i(G)$ ($i = 0, 1, \ldots, n$) for UOB graphs. This in turn provides a way of comparing the energies of a pair of UOB graphs. That is to say, the method of the quasi-ordering relation "$\preccurlyeq$" defined by Gutman and Polansky [4] on the set of forests can now be generalized to the set of UOB graphs as follows:

Definition 1.1. Let G_1 and G_2 be two UOB graphs of order n. If $b_i(G_1) \leqslant b_i(G_2)$ for all i with $2 \leqslant i \leqslant n$, then we write that $G_1 \preccurlyeq G_2$. (Note that $b_0(G) = 1$ and $b_1(G) = 0$ for all graphs G.)

Furthermore, if $G_1 \preccurlyeq G_2$ and there exists at least one index j such that $b_j(G_1) < b_j(G_2)$, then we write that $G_1 \prec G_2$.

If $b_i(G_1) = b_i(G_2)$ for all i (i.e., if $G_1 \preccurlyeq G_2 \preccurlyeq G_1$), we write $G_1 \sim G_2$.

According to the Coulson integral formula (1.2), we have for two UOB graphs G_1 and G_2 of order n that

$$G_1 \preccurlyeq G_2 \Longrightarrow E(G_1) \leqslant E(G_2),$$

and

$$G_1 \prec G_2 \Longrightarrow E(G_1) < E(G_2).$$

In this paper, we study how graph energies change under certain graph operations on UOB graphs. We will show in Section 3 that for two UOB graphs one of which is obtained from the other by applying an "edge grafting" operation, the quasi-order relation between them is totally determined by the parity of the shortest length among those relevant pendant paths. As an application, we determine (in Section 4) the maximal and minimal energy graph among all the graphs obtained by attaching some rooted tree of fixed order to some vertex u of some UOB graph G.

2. A recurrence relation of the quasi-orders upon deleting a cut edge on unicyclic or bipartite graphs

In this section, we will give a generalization (in Lemma 2.3) of a well known recurrence relation on the quasi-orders from acyclic graphs to UOB graphs. This result will be used throughout the paper.

The following lemma is another form of Theorem 2.12 in [1]. We write down a short proof here for the self-contained purpose of the paper.

Lemma 2.1. *Let uv be a cut edge of a graph G. Then we have*

$$\phi(G,x) = \phi(G-uv,x) - \phi(G-u-v,x).$$

Proof. Write $G - uv = G_1 \cup G_2$, where $G_1,\ G_2$ are graphs of order $n_1,\ n_2$ with adjacency matrices $A_1,\ A_2$, respectively. Without loss of generality, we may assume that u is the last vertex of G_1, and v is the first vertex of G_2. Let E_1 be the $n_1 \times n_2$ matrix with the $(n_1, 1)$ entry be 1 and all the other entries zero, and e_1 be the last row of E_1. Then we have:

$$\begin{aligned}\phi(G,x) &= \mathbf{det}(xI-A) = \mathbf{det}\begin{pmatrix} xI_{n_1}-A_1 & -E_1 \\ -E_1^T & xI_{n_2}-A_2 \end{pmatrix} \\ &= \mathbf{det}\begin{pmatrix} xI_{n_1}-A_1 & O \\ -E_1^T & xI_{n_2}-A_2 \end{pmatrix} + \mathbf{det}\begin{pmatrix} xI_{n_1-1}-A(G_1-u) & * & O \\ 0 \ \cdot \ \cdot \ \cdot \ 0 & 0 & -e_1 \\ O & -e_1^T & xI_{n_2}-A_2 \end{pmatrix} \\ &= \phi(G_1,x)\phi(G_2,x) - \phi(G_1-u,x)\phi(G_2-v,x) = \phi(G-uv,x) - \phi(G-u-v,x). \quad \square\end{aligned}$$

From Lemma 2.1, we can get the following recurrence relation of $b_i(G)$ for UOB graphs. This result for the unicyclic graphs in the special case of the pendant edge can also be found in [5,6].

Lemma 2.2. *Let uv be a cut edge of a UOB graph G. Then we have*:

$$b_i(G) = b_i(G-uv) + b_{i-2}(G-u-v) \quad (i \geqslant 2). \tag{2.1}$$

Proof. By Lemma 2.1, we have

$$\sum_{i=0}^{n} a_i(G)x^{n-i} = \sum_{i=0}^{n} a_i(G-uv)x^{n-i} - \sum_{i=0}^{n-2} a_i(G-u-v)x^{n-i-2}.$$

Comparing the coefficients of x^{n-i} for both sides of the above equation, we have

$$a_i(G) = a_i(G-uv) - a_{i-2}(G-u-v). \tag{2.2}$$

Case 1: i is even, say $i = 2j$.

Multiplying both sides of (2.2) by $(-1)^j$, and using result (1) of Lemma 1.1, we obtain (2.1).

Case 2: i is odd, say $i = 2j + 1$.

If G is bipartite, then all the three terms of (2.1) are zero. So in this case we may assume that G is unicyclic containing a (single) cycle C of length l.

Subcase 2.1: $G - u - v$ contains no cycle. Then it is a forest, and thus $a_{i-2}(G-u-v) = 0 = b_{i-2}(G-u-v)$. So (2.2) implies $a_i(G) = a_i(G-uv)$. Taking the absolute values for both sides, we obtain $b_i(G) = b_i(G-uv) = b_i(G-uv) + b_{i-2}(G-u-v)$.

Subcase 2.2: $G - u - v$ contains the cycle C. Then both $G - uv$ and $G - u - v$ are single-cycle graphs (containing the same cycle C).

Multiplying both sides of (2.2) by $(-1)^j$, we obtain

$$(-1)^j a_{2j+1}(G) = (-1)^j a_{2j+1}(G - uv) + (-1)^{j-1} a_{2j-1}(G - u - v). \tag{2.3}$$

By using the result (2) or (3) of Lemma 1.1, we can see that the two terms of the right side of (2.3) can not have the opposite signs (since the cycle in $G - uv$ and in $G - u - v$ have the same length l). Thus taking the absolute values for both sides of (2.3), we obtain (2.2). □

From Lemma 2.2 we can get the following useful corollary which will be used in Sections 3 and 4.

Corollary 2.1. *Let uv be a cut edge of a UOB graph G. Then we have* $G - uv \prec G$.

Proof. By Lemma 2.2 we have $b_i(G) - b_i(G - uv) = b_{i-2}(G - u - v) \geqslant 0$ for $i \geqslant 2$.

On the other hand, we have $b_2(G) > b_2(G - uv)$ since G obviously have more edges than $G - uv$. So we have $G - uv \prec G$. □

From Lemma 2.2 we can also directly obtain the following recurrence relation on the quasi-orders of UOB graphs.

Lemma 2.3. *Let uv (respectively, $u'v'$) be a cut edge of a UOB graph G (respectively, G'). Suppose that* $G - uv \preccurlyeq G' - u'v'$ *and* $G - u - v \preccurlyeq G' - u' - v'$, *then we have* $G \preccurlyeq G'$, *with* $G \sim G'$ *if and only if both the two relations* $G - uv \sim G' - u'v'$ *and* $G - u - v \sim G' - u' - v'$ *hold.*

An important and frequently used special case of Lemma 2.3 is that u (respectively, u') is a pendant vertex of G (respectively, G'). Then in this case we have $G - uv \preccurlyeq G' - u'v' \Longleftrightarrow G - u \preccurlyeq G' - u'$.

3. The effect of edge-graftings on the quasi-orders of UOB graphs

Let u, v be two vertices (not necessarily distinct) in a graph G, and a, b be two non-negative integers. Let $G_{u,v}(a, b)$ be the graph obtained by attaching to G two (new) pendent paths of lengths a and b at u and v, respectively (see Fig. 1). Also, we sometimes use $G_{u,v}$ to denote a graph G with two vertices u and v specified.

When $a + b = c + d$ (where a, b, c, d are non-negative integers), we say that the graph $G_{u,v}(c, d)$ is obtained from $G_{u,v}(a, b)$ by an "edge grafting" operation (on the two relevant pendant paths of $G_{u,v}(a, b)$).

The edge grafting operations on the trees were often considered and used in the study of the spectra of graphs. Recently [7], we also used the special case $u = v$ of the edge grafting to study the quasi-order relations and the comparison of graph energies between trees. In this section, we will study the effect of the edge grafting operations on the quasi-orders and graph energies for UOB graphs.

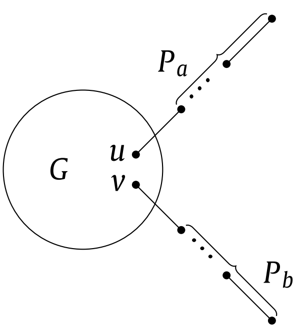

Fig. 1. The graph $G_{u,v}(a, b)$.

We first consider a "total edge grafting" for the general case where u may not equal to v, and even the two graphs G and H in the following Lemma 3.1 may not be the same.

Lemma 3.1. *Let u, v be two vertices of a UOB graph G, s, t be two vertices of a UOB graph H. If G and H satisfy:*

(1) $G_{u,v}(0,2) \succ H_{s,t}(1,1)$.
(2) $G_{u,v}(0,1) \succcurlyeq H_{s,t}(0,1)$.
(3) *For any positive integer p,* $G_{u,v}(0,p) \succcurlyeq H_{s,t}(p,0)$.

Then for any positive integers a, b, we have $G_{u,v}(0,a+b) \succ H_{s,t}(a,b)$.

Proof. Case 1: $b = 1$. We use induction on a.

If $a = 0$, then we have $G_{u,v}(0,a+b) \succcurlyeq H_{s,t}(a,b)$ by condition (2). If $a = 1$, then the result holds by condition (1).

In general when $a \geqslant 2$, take the pendant edge in the pendant path of length $a+1$ of $G_{u,v}(0,a+b)$, and the pendant edge in the pendant path of length a of $H_{s,t}(a,b)$ as the cut edges, respectively, then use Lemma 2.3 and the inductive hypothesis on a, we have:

$$G_{u,v}(0,a) \succ H_{s,t}(a-1,1), \quad G_{u,v}(0,a-1) \succcurlyeq H_{s,t}(a-2,1) \Longrightarrow G_{u,v}(0,a+1) \succ H_{s,t}(a,1).$$

Case 2: $b \geqslant 2$. We use induction on b.

If $b = 0$, then we have $G_{u,v}(0,a+b) \succcurlyeq H_{s,t}(a,b)$ by condition (3). If $b = 1$, then the result hold by Case 1.

In general when $b \geqslant 2$, take the pendant edge in the pendant path of length $a+b$ of $G_{u,v}(0,a+b)$, and the pendant edge in the pendant path of length b of $H_{s,t}(a,b)$, respectively. Then by the inductive hypothesis on b we have:

$$G_{u,v}(0,a+b-1) \succ H_{s,t}(a,b-1), \quad G_{u,v}(0,a+b-2) \succcurlyeq H_{s,t}(a,b-2),$$

which imply $G_{u,v}(0,a+b) \succ H_{s,t}(a,b)$ by using Lemma 2.3. □

The following Lemma 3.2 will only be used in the proof of Theorem 3.1.

Lemma 3.2. *Let u, v be two vertices of a UOB graph G satisfying $G_{u,v}(0,2) \succ G_{u,v}(1,1)$, then we have:*

(1) *For any integer $k \geqslant 0$, we have*

$$G_{u,v}(2k,2k+2) \succ G_{u,v}(2k+1,2k+1).$$

(2) *For any integer $k \geqslant 0$, we have*

$$G_{u,v}(2k+2,2k+2) \succ G_{u,v}(2k+1,2k+3).$$

Proof. (1) We use induction on k. If $k = 0$, then the result holds by the hypothesis. So we assume that $k \geqslant 1$. By the inductive hypothesis we have

$$G_{u,v}(2k-2,2k) \succ G_{u,v}(2k-1,2k-1).$$

First we prove the following relation (3.1):

$$G_{u,v}(2k,2k) \succ G_{u,v}(2k-1,2k+1). \tag{3.1}$$

Take the pendant vertex x and pendant edge xy in the pendant path of length $2k$ (starting from u) of $G_{u,v}(2k,2k)$, and the pendant vertex x' and pendant edge $x'y'$ in the pendant path of length $2k+1$ of $G_{u,v}(2k-1,2k+1)$, respectively, and then use the inductive hypothesis on k, we have:

$$\begin{aligned} G_{u,v}(2k,2k) - x &= G_{u,v}(2k-1,2k) = G_{u,v}(2k-1,2k+1) - x', \\ G_{u,v}(2k,2k) - x - y &= G_{u,v}(2k-2,2k) \succ G_{u,v}(2k-1,2k-1) \\ &= G_{u,v}(2k-1,2k+1) - x' - y'. \end{aligned}$$

Using these two relations and Lemma 2.3, we obtain (3.1).

Next, take the pendant vertex x and pendant edge xy in the pendant path of length $2k+2$ of $G_{u,v}(2k, 2k+2)$, and the pendant vertex x' and pendant edge $x'y'$ in the pendant path of length $2k+1$ (starting from u) of $G_{u,v}(2k+1, 2k+1)$, respectively, we have:

$$\begin{aligned} G_{u,v}(2k, 2k+2) - x &= G_{u,v}(2k, 2k+1) = G_{u,v}(2k+1, 2k+1) - x', \\ G_{u,v}(2k, 2k+2) - x - y &= G_{u,v}(2k, 2k) \succ G_{u,v}(2k-1, 2k+1) \\ &= G_{u,v}(2k+1, 2k+1) - x' - y' \quad \text{by (3.1)}. \end{aligned}$$

Using these two relations and Lemma 2.3, we obtain the result (1).

(2) Similarly, take the pendant vertex x and pendant edge xy in the pendant path of length $2k+2$ (starting from u) of $G_{u,v}(2k+2, 2k+2)$, and the pendant vertex x' and pendant edge $x'y'$ in the pendant path of length $2k+3$ of $G_{u,v}(2k+1, 2k+3)$, respectively, we have:

$$\begin{aligned} G_{u,v}(2k+2, 2k+2) - x &= G_{u,v}(2k+1, 2k+2) = G_{u,v}(2k+1, 2k+3) - x', \\ G_{u,v}(2k+2, 2k+2) - x - y &= G_{u,v}(2k, 2k+2) \succ G_{u,v}(2k+1, 2k+1) \\ &= G_{u,v}(2k+1, 2k+3) - x' - y'. \end{aligned}$$

Using these two relations and Lemma 2.3, we obtain the result (2). □

The following Theorem 3.1 concerns a kind of edge grafting for the two pairs of pendant paths rooted at two (possibly distinct) vertices u and v. Here the result (2) of Theorem 3.1 will only be used in the proof of result (3) of Theorem 3.1.

Theorem 3.1. *Let u, v be two vertices of UOB graph G. Suppose that G satisfies:*

(*i*) $G_{u,v}(0, 2) \succ G_{u,v}(1, 1)$.
(*ii*) *For any non-negative integers p, q, we have $G_{u,v}(p, q) = G_{u,v}(q, p)$.*

Let a, b, c, d be non-negative integers with $a \leqslant b$, $c \leqslant d$, $a + b = c + d$, and $a < c$, then we have:

(*1*) *If a is even, then $G_{u,v}(a, b) \succ G_{u,v}(c, d)$.*
(*2*) *If both k, j are not equal to 1, then $G_{u,v}(1, k+j-1) \prec G_{u,v}(k, j)$.*
(*3*) *If a is odd, then $G_{u,v}(a, b) \prec G_{u,v}(c, d)$.*

Proof. (1) Write $a = 2k$. Take $H = G_{u,v}(a, a)$, let s, t be the pendant vertices of the two pendant paths of length a of H. Then by condition (ii) we have:

$$H_{s,t}(p, q) = G_{u,v}(a+p, a+q) = G_{u,v}(a+q, a+p) = H_{s,t}(q, p).$$

By Lemma 3.2 we also have:

$$\begin{aligned} G_{u,v}(0, 2) \succ G_{u,v}(1, 1) &\Longrightarrow G_{u,v}(2k, 2k+2) \succ G_{u,v}(2k+1, 2k+1) \\ &\Longrightarrow H_{s,t}(0, 2) \succ H_{s,t}(1, 1). \end{aligned}$$

Thus $H_{s,t}$ satisfies all the conditions of Lemma 3.1 (take $G_{u,v}$ in Lemma 3.1 to be $H_{s,t}$). So use Lemma 3.1 for $H_{s,t}$, we can obtain $H_{s,t}(0, b-a) \succ H_{s,t}(c-a, d-a)$, and this is the same as our desired result $G_{u,v}(a, b) \succ G_{u,v}(c, d)$.

(2) If one of k, j is zero, then (2) follows directly from (1). So in the following we assume that $k, j \geqslant 2$. Now we use induction on k. If $k = 0$, the result holds by the previous result (1). If $k = 1$, then we obviously have $G_{u,v}(1, k+j-1) = G_{u,v}(k, j)$. Now the general case follows from Lemma 2.3 and the induction on k, by taking the pendant edge in the pendant path of length $k+j-1$ of $G_{u,v}(1, k+j-1)$, and the pendant edge in the pendant path of length k of $G_{u,v}(k, j)$, respectively.

(3) By result (2) we may assume that $a = 2k+1 \geqslant 3$. Take $H = G_{u,v}(2k, 2k)$. Then similar to (1) we can check that $H_{s,t}$ satisfies the conditions (i) and (ii) of this theorem for $G_{u,v}$. So the result (2) of

this theorem also holds for $H_{s,t}$, namely we have $H_{s,t}(1, b-2k) \prec H_{s,t}(c-2k, d-2k)$, and this is the same as our desired result $G_{u,v}(a,b) \prec G_{u,v}(c,d)$. $\square$

Next we are going to show (in Corollary 3.1) that if $u = v$ and v is a non-isolated vertex of a UOB graph G, then the condition (i) of Theorem 3.1 can always be satisfied. For this purpose, we need first to prove the following Lemmas 3.3 and 3.4. The proof of Lemma 3.3 will also need to use the following well known Sachs Theorem [1].

Let $\mathfrak{L}_i(G)$ be the set of subgraphs with order i of G each of whose components is either a single edge or a single cycle, then the well-known Sachs Theorem gives:

$$a_i(G) = \sum_{S \in \mathfrak{L}_i(G)} (-1)^{p(S)} 2^{c(S)}, \tag{3.2}$$

where $p(S)$ is the number of components of S and $c(S)$ is the number of cycles of S.

Recalling that $G_1(n,l)$ denotes the set of single-cycle graphs of order n whose unique cycle has length l.

Now let $G \in G_1(n,l)$ with a single cycle C of length l.

Let $m(G,k)$ be the number of k-matchings of G, and we assume that $m(G,k) = 0$ if k is not a non-negative integer.

Lemma 3.3. *Let $G \in G_1(n,l)$ with a single cycle C of odd length l, $e = uv$ be an edge of G. Then we have $G \succ G - e$.*

Proof. If $e = uv$ is a cut edge of G, then the result follows directly from Corollary 2.1. So we may assume that the edge e is on the cycle C. In this case, $G - e$ is a forest, so by Sachs Theorem we have $b_i(G-e) = m\left(G-e, \frac{i}{2}\right)$. Now we consider two cases.

Case 1: i is odd. Then $b_i(G-e) = 0 \leqslant b_i(G)$.

Case 2: i is even. Now l is odd. Then each subgraph in $\mathfrak{L}_i(G)$ does not contain the unique cycle C of G, and thus must be an $\frac{i}{2}$-matching of G. So we have

$$a_i(G) = \sum_{S \in \mathfrak{L}_i(G)} (-1)^{p(S)} 2^{c(S)} = (-1)^{\frac{i}{2}} m\left(G, \frac{i}{2}\right)$$

and so $b_i(G) = |a_i(G)| = m\left(G, \frac{i}{2}\right) \geqslant m\left(G-e, \frac{i}{2}\right) = b_i(G-e)$.

Combining the above two cases, we always have $b_i(G) \geqslant b_i(G-e)$.

On the other hand, it is obvious that $b_2(G) = |E(G)| > |E(G-e)| = b_2(G-e)$. From this we obtain that $G \succ G - e$. $\square$

Lemma 3.4. *Let v be a non-isolated vertex in a UOB graph G, K_1 be the trivial graph of order 1. Then $G \succ (G-v) \cup K_1$.*

Proof. Case 1: G is a bipartite graph. Then $(G-v) \cup K_1$ is also a bipartite graph.

Let $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_n$ be the eigenvalues of G with $\mu_s > 0 \geqslant \mu_{s+1}$, $\lambda_1' \geqslant \lambda_2' \geqslant \cdots \geqslant \lambda_{n-1}'$ be the eigenvalues of $G - v$, and $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of $(G-v) \cup K_1$. By the Cauchy interlacing theorem, we have $\lambda_{s-1}' \geqslant \mu_s > 0 \geqslant \mu_{s+1} \geqslant \lambda_{s+1}'$.

On the other hand, the spectrum of $G - v$ can be obtained by deleting an eigenvalue 0 from the spectrum of $(G-v) \cup K_1$, so we have $\lambda_{s+1} \leqslant \mathrm{Max}\{\lambda_{s+1}', 0\} \leqslant 0$, and $0 \leqslant \lambda_s = \mathrm{Max}\{\lambda_s', 0\} \leqslant \mu_s$.

Since G and $(G-v) \cup K_1$ are both bipartite graphs, We get the following formulas:

$$\phi(G,x) = x^{n-2s} \prod_{i=1}^{s} \left(x^2 - \mu_i^2\right), \quad \phi((G-v) \cup K_1, x) = x^{n-2s} \prod_{i=1}^{s} \left(x^2 - \lambda_i^2\right),$$

where $\mu_i \geqslant \lambda_i' = \lambda_i > 0$ for $i = 1, \ldots, s-1$, and $\mu_s \geqslant \lambda_s \geqslant 0$.

Now using Viète's formulas on the relations between roots and coefficients of polynomials, we get:

$$b_{2k}(G)=\sum_{1\leqslant i_1<i_2<\cdots<i_k\leqslant s}(\mu_{i_1}\mu_{i_2}\cdots\mu_{i_k})^2,\qquad b_{2k}((G-v)\cup K_1)=\sum_{1\leqslant i_1<i_2<\cdots<i_k\leqslant s}(\lambda_{i_1}\lambda_{i_2}\cdots\lambda_{i_k})^2.$$

It follows from this that $b_i(G)\geqslant b_i((G-v)\cup K_1)$ for all i. Since v is a non-isolated vertex of G, the edge set of $(G-v)\cup K_1$ is a proper subset of the edge set of G. Then $b_2(G)=|E(G)|>|E((G-v)\cup K_1)|=b_2((G-v)\cup K_1)$, so we obtain $G\succ(G-v)\cup K_1$.
Case 2: G is a unicyclic graph with the cycle length l.
Subcase 2.1: l is even. Then G is a bipratite graph, and the result follows from Case 1.
Subcase 2.2: l is odd. Since v is a non-isolated vertex of G, $(G-v)\cup K_1$ is a proper spanning subgraph of G. So by Lemma 3.3 we have $G\succ(G-v)\cup K_1$. □

Now we can show that if $u=v$ and v is a non-isolated vertex of a UOB graph G, then the condition (i) of Theorem 3.1 can always be satisfied.

Corollary 3.1. *Let v be a non-isolated vertex in a UOB graph G. Then we have $G_{v,v}(0,2)\succ G_{v,v}(1,1)$.*

Proof. Let $e=xy$ be the pendant edge (with pendant vertex x) on the pendant path of length 2 of $G_{v,v}(0,2)$, and $e'=x'y'$ be the pendant edge (with pendant vertex x' and $y'=v$) on a pendant path of length 1 of $G_{v,v}(1,1)$. Then we have:

$$G_{v,v}(0,2)-x=G_{v,v}(0,1)=G_{v,v}(1,1)-x' \tag{3.2}$$

and

$$G_{v,v}(0,2)-x-y=G_{v,v}(0,0)=G,\qquad G_{v,v}(1,1)-x'-y'=G_{v,v}(0,1)-v=(G-v)\cup K_1.$$

By Lemma 3.4 we have

$$G_{v,v}(0,2)-x-y\succ G_{v,v}(1,1)-x'-y'. \tag{3.3}$$

Combining (3.2) and (3.3) and using Lemma 2.3 we obtain $G_{v,v}(0,2)\succ G_{v,v}(1,1)$. □

Combining Theorem 3.1 and Corollary 3.1, we can now obtain the following result on the quasi-orders of two UOB graphs one of which is obtained from the other by an edge grafting operation.

Theorem 3.2. *Let v be a non-isolated vertex of a UOB graph G. Let a,b,c,d be non-negative integers with $a\leqslant b,\ c\leqslant d,\ a+b=c+d$, and $a<c$. Then we have*:

(*1*) *If a is even, then $G_{v,v}(a,b)\succ G_{v,v}(c,d)$.*
(*2*) *If a is odd, then $G_{v,v}(a,b)\prec G_{v,v}(c,d)$.*

Proof. From Corollary 3.1 we see that $G_{v,v}$ satisfies the two conditions of Theorem 3.1 (with $u=v$). So the results follow from Theorem 3.1. □

In the special case when $a=0$, we have $G_{v,v}(0,c+d)\succ G_{v,v}(c,d)$ when $0<c\leqslant d$. This special case is called a total edge grafting at the same vertex.

4. Some applications

In this section, we will give some applications of the above results (about the effect of edge grafting on the quasi-orders of UOB graphs) to the comparison of the energies of some unicyclic and bipartite graphs.

Let u be a vertex of a graph G, and T be a rooted tree. Let $G_u(T)$ denote the graph obtained by attaching T to G such that the root of T is at u. When T is a path P_{k+1} with one of its ends as the root, then we simply write $G_u(T)$ as $G_u(k)$. When T is a star $K_{1,k}$ with the center as its root, then we simply write $G_u(T)$ as $G^*_u(k)$.

Theorem 4.1. *Let u be a vertex of a UOB graph G and T be a tree of order $k+1$ rooted at u. Then we have:*

(1) *If $G_u(T) \neq G_u(k)$, then $G_u(T) \prec G_u(k)$.*
(2) *If $G_u(T) \neq G_u^*(k)$, then $G_u(T) \succ G_u^*(k)$.*

Proof. If u is an isolated vertex of G, then the results follow from the well known results of trees. So in the following we assume that u is a non-isolated vertex of G.

(1) Let r be the number of vertices of degree at least 3 in T different from u. We use induction on r. If $r = 0$, Then T consists of some (say, i) pendant paths starting from u. Since $G_u(T) \neq G_u(k)$, we have $i \geqslant 2$. Now by using $(i-1)$-times "total edge graftings" for $G_u(T)$ at u, we can get $G_u(k)$. Thus using Corollary 3.1 we obtain $G_u(T) \prec G_u(k)$.

Now we assume $r \geqslant 1$. Let v be a vertex of T with degree at least 3 which is furthest to u. Then there are $(d(v)-1)$ many pendant paths starting from v. By using $(d(v)-2)$ many "total edge graftings" on these pendant paths at v, we can obtain a $G_u(T')$ where the tree T' (rooted at u) contains $(r-1)$ vertices of degree at least 3 different from u. So by using Corollary 3.1 and the inductive hypothesis we have $G_u(T) \prec G_u(T') \preccurlyeq G_u(k)$.

(2) We use induction on k.

If $k = 2$, then the result follows from the result (1) of this theorem. Now we assume $k \geqslant 3$.

Let x be a pendent vertex in $G_u^*(k)$ and let $y = u$. Then we have

$$G_u^*(k) - x = G_u^*(k-1), \quad G_u^*(k) - x - y = (G-u) \cup (k-1)K_1. \tag{4.1}$$

Since $G_u(T) \neq G_u^*(k)$, there exists at least one non-pendant vertex in T different from u. Let y' be a non-pendant vertex of T which is furthest to u. Then there are $(d(y')-1)$ many pendant vertices adjacent to y'. Let x' be a pendant vertex adjacent to y'. Then we have:

$$G_u(T) - x' = G_u(T-x'), \quad G_u(T) - x' - y' = G_u(T-x') - y' = G_u(T') \cup (d(y')-2)K_1, \tag{4.2}$$

where T' is some tree of order $k+1-d(y')$ rooted at u.

Let E' be the edge set of the tree T'. Since every edge of T' is a cut edge of $G_u(T')$, by Corollary 2.1 we have $G_u(T') \succcurlyeq G_u(T') - E' = G \cup (k-d(y'))K_1$. It follows from this and Lemma 3.4 that

$$G_u^*(k) - x - y = (G-u) \cup (k-1)K_1 = (G-u) \cup K_1 \cup (k-d(y'))K_1 \cup (d(y')-2)K_1$$

$$\prec G \cup (k-d(y'))K_1 \cup (d(y')-2)K_1 \preccurlyeq G_u(T') \cup (d(y')-2)K_1 = G_u(T) - x' - y'.$$

On the other hand, by induction we have

$$G_u^*(k) - x = G_u^*(k-1) \preccurlyeq G_u(T-x') = G_u(T) - x'$$

Thus by using Lemma 2.3 we have $G_u(T) \succ G_u^*(k)$. □

Now let $G^*(n,l)$ be the set of unicyclic graphs in $G(n,l)$ such that all the trees attached to the cycle C_l are paths rooted at one of their ends. It is easy to see that $G \in G^*(n,l)$ if and only if G satisfies the following three conditions:

(1) $G \in G(n,l)$.
(2) $\Delta(G) \leqslant 3$.
(3) All the vertices of degree 3 of G (if any) are on the cycle C_l.

The following corollary follows directly from Theorem 4.1 which tells that the graph in $G(n,l)$ with the greatest energy must be in $G^*(n,l)$.

Corollary 4.1. *Let $G \in G(n,l) \backslash G^*(n,l)$. Then there exists some graph $H \in G^*(n,l)$ such that $G \prec H$.*

The result in the following Example 4.1 was obtained in [6]. Here we give a short proof of this result by using Corollary 4.1 and our edge grafting result for two pairs of pendant paths rooted at different vertices in Theorem 3.1.

Example 4.1. Let P_n^3 be the unicyclic graph of order n obtained by identifying a vertex of the cycle C_3 with an end vertex of the path P_{n-2}. Then P_n^3 is the graph with the greatest energy in $G(n, 3)$.

Proof. Let G be any graph in $G(n, 3)$ with $G \neq P_n^3$.

Case 1: $G \in G^*(n, 3)$.

Let v_1, v_2, v_3 be the three vertices on the cycle of G, and there is a pendant path Q_i of length a_i attached to v_i $(i = 1, 2, 3)$, where a_1, a_2, a_3 are integers with $0 \leqslant a_1 \leqslant a_2 \leqslant a_3$. We denote this graph G by $C_3(a_1, a_2, a_3)$. Since $G \neq P_n^3$, we have $a_2 > 0$.

Let H be the graph obtained from G by deleting all the vertices of Q_2 and Q_3 except v_2 and v_3, then we have $G = H_{v_2,v_3}(a_2, a_3)$. It is now easy to check that H_{v_2,v_3} satisfies the two conditions on $G_{u,v}$ in Theorem 3.1:

(i) Using Lemmas 2.3 and 3.3 we can check that $H_{v_2,v_3}(0, 2) \succcurlyeq H_{v_2,v_3}(1, 1)$.

(ii) It is obvious that $H_{v_2,v_3}(p, q) = H_{v_2,v_3}(q, p)$.

So by using Theorem 3.1, we obtain

$$G = C_3(a_1, a_2, a_3) \prec C_3(a_1, 0, a_2 + a_3) \preccurlyeq C_3(0, 0, a_1 + a_2 + a_3) = P_n^3.$$

Case 2: $G \notin G^*(n, 3)$. Then by Corollary 4.1 we know that there exists a graph $H \in G^*(n, 3)$ such that $G \prec H$. So by Case 1 we have $G \prec H \preccurlyeq P_n^3$. □

References

[1] Dragos M. Cvetkovic, Michael Doob, Horst Sachs, Spectra of Graphs: Theory and Applications (Pure and Applied Mathematics), third revised ed., vol. 8, Academic Press, 1997.
[2] I. Gutman, The energy of a graph, Ber. Math.-Statist. Sekt. Forsch. Graz 103 (1978) 1–22.
[3] I. Gutman, The Energy of a Graph: Old and New Results, Algebraic Combinatorics and Applications, Springer-Verlag, Berlin, 2001, pp. 196–211.
[4] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin, 1986.
[5] Yaoping Hou, Unicyclic graphs with minimal energy, J. Math. Chem. 29 (3) (2001) 163–168.
[6] Yaoping Hou, I. Gutman, Ching-Wah Woo, Unicyclic graphs with maximal energy, Linear Algebra Appl. 356 (2002) 27–36.
[7] Hai-ying Shan, Jia-yu Shao, Graph energy change due to edge grafting operations and its applications, Match Commun. Math. Comput. Chem. 64 (2010) 25–40.