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EDGE-GRAFTING THEOREMS ON PERMANENTS OF THE LAPLACIAN MATRICES OF GRAPHS AND THEIR APPLICATIONS*

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Abstract. The trees, respectively unicyclic graphs, on n vertices with the smallest Laplacian permanent are studied. In this paper, by edge-grafting transformations, the n-vertex trees of given bipartition having the second and third smallest Laplacian permanent are identified. Similarly, the n-vertex bipartite unicyclic graphs of given bipartition having the first, second and third smallest Laplacian permanent are characterized. Consequently, the n-vertex bipartite unicyclic graphs with the first, second and third smallest Laplacian permanent are determined.

Key words. Laplacian matrix, Laplacian coefficient, Permanent, Tree, Unicyclic graph, Bipartition.

AMS subject classifications. 05C50, 05C05.

1. Introduction.

Let $G = (V_G, E_G)$ be a simple connected graph with vertex set $V_G = \{v_1, \ldots, v_n\}$ and edge set $E_G \neq \emptyset$. The adjacency matrix $A(G) = (a_{ij})$ of G is an $n \times n$ symmetric matrix with $a_{ij} = 1$ if and only if v_i, v_j are adjacent and 0 otherwise. Since G has no loops, the main diagonal of $A(G)$ contains only 0's. Denote the degree of v_i by $d_G(v_i)$ (or d_i) for $i = 1, \ldots, n$, and let $D(G)$ be the diagonal matrix whose (i,i)-entry is $d_i, i = 1, 2, \ldots, n$. The matrix $L(G) = D(G) - A(G)$ is called the *Laplacian matrix* of G. Of course, $L(G)$ depends on the ordering of the vertices of G. However, a different ordering leads to a matrix which is permutation similar to $L(G)$. The matrix $Q(G) = D(G) + A(G)$ has been called the *signless Laplacian matrix* of G. For survey papers on this matrix the reader is referred to [2, 3, 4].

If the vertex set of the connected graph G on n vertices can be partitioned into two subsets V_1 and V_2 such that each edge joins a vertex of V_1 to a vertex of V_2, then G has a (p,q)-*bipartition* where $|V_1| = p$ and $|V_2| = q$. Without loss of generality we may assume that $p \leq q$.

A connected graph with n vertices and n edges is called a *unicyclic graph*. For convenience, let $\mathscr{T}_n^{p,q}$ (resp., $\mathscr{U}_n^{p,q}$) be the set of all n-vertex trees (resp., bipartite unicyclic graphs) with a (p,q)-bipartition, and let $\mathscr{U}_n$ be the set of all bipartite unicyclic graphs on n vertices.

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Throughout we denote by P_n, S_n and C_n the path, star and cycle on n vertices, respectively. Let $G-v, G-uv$ denote the graph obtained from G by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G+uv$ is obtained from G by adding edge $uv \notin E_G$. The *distance* between vertices u and v in G is denoted by $d_G(u,v)$. Let $PV(G)$ denote the set of all pendant vertices of G.

The *permanent* of $X=(x_{ij}) \in M_{n\times n}$, denoted by per$X$, is the quantity

$$\mathrm{per}X = \sum_{\sigma\in S_n}\prod_{t=1}^{n} x_{t\sigma(t)},$$

where S_n is the symmetric group of degree n; see [16]. It was suggested in [15] to use the polynomial per$(xI-L(G))$ to distinguish non-isomorphic trees. For more progress on the quantity per$(\cdot)$, the reader is referred to [19].

The first research paper on the permanent of the Laplacian matrix was [15], in which lower bounds for the permanent of $L(G)$ were conjectured by Merris, Rebman and Watkins. These lower bounds on per$L(G)$ were proved by Brualdi and Goldwasser [1] and Merris [14]. For more recent results on Laplacian (resp., signless Laplacian) permanent one is referred to [5, 11, 12].

The Laplacian polynomial $\mu(G,\lambda)$ of G is the *characteristic polynomial* of its Laplacian matrix $L(G)$, that is,

$$\mu(G,\lambda) = \det(\lambda I_n - L(G)) = \sum_{k=0}^{n}(-1)^k c_k \lambda^{n-k}.$$

It is easy to see that $c_0(G)=1, c_1(G)=2|E_G|, c_n(G)=0, c_{n-1}(G)=n\tau(G)$, where $\tau(G)$ denotes the number of spanning trees of G. For two n-vertex graphs G_1 and G_2, we say that G_1 is dominated by G_2 and write $G_1 \preceq G_2$, if $c_k(G_1) \le c_k(G_2)$ holds for all Laplacian coefficients $c_k, k=0,1,\ldots,n$. If $G_1 \preceq G_2$ and there exists j such that $c_j(G_1) < c_j(G_2)$, then we write $G_1 \prec G_2$.

Note that the Laplacian coefficients have combinatorial significance, hence the research on the Laplacian coefficients of graphs has received great attention in recent years; see [6, 7, 8, 9, 10, 17, 18, 20] and the references therein. Zhou and Gutman [21] showed that among all trees of order n, the kth coefficient c_k is the largest when the tree is a path and is the smallest for a star, $k=0,1,\ldots,n$. In view of Theorems 2.4 and 2.5 in [1] the counterparts of these results for the Laplacian permanent of trees are as follows.

THEOREM 1.1 ([1]). *Let T be a tree with n vertices. Then*

$$2(n-1) \le \mathrm{per}\ L(T) \le \frac{2-\sqrt{2}}{2}(1+\sqrt{2})^n + \frac{2+\sqrt{2}}{2}(1-\sqrt{2})^n.$$

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The left equality holds if and only if T is a star, whereas the right equality holds if and only if T is a path.

Brualdi and Goldwasser [1] showed that $T_{n,m}$ is the unique tree among the n-vertex trees each of which contains an m-matching having the minimum Laplacian permanent, where $T_{n,m}$ is the tree obtained from the star graph S_{n-m+1} by attaching a pendant edge to each of certain $m-1$ non-central vertices of S_{n-m+1}. Ilić [8] showed that $T_{n,m}$ is also the unique n-vertex tree with given matching number m which simultaneously minimizes all the Laplacian coefficients. It is then natural to conjecture that among the class of graphs, if a particular graph has the smallest Laplacian permanent, then that particular graph also minimizes all of its Laplacian coefficients in that class of graphs, and vice versa. This mathematical phenomenon is further studied in [1, 7]. We know from [7] that among the n-vertex trees of diameter d, the caterpillar $T_{n,d,\lfloor d/2\rfloor}$ has the minimum Laplacian coefficient c_k, for every $k = 0, 1, \ldots, n$, whereas we know from [1] that among the n-vertex trees of diameter d, the broom $T_{n,d,2}$ has the minimum Laplacian permanent. Graphs $T_{n,d,\lfloor d/2\rfloor}$ and $T_{n,d,2}$ are depicted in Fig. 1.1. This implies that there is no monotone relationship between the Laplacian coefficients and the Laplacian permanent of graphs. Yet we lack a better understanding of this relationship.

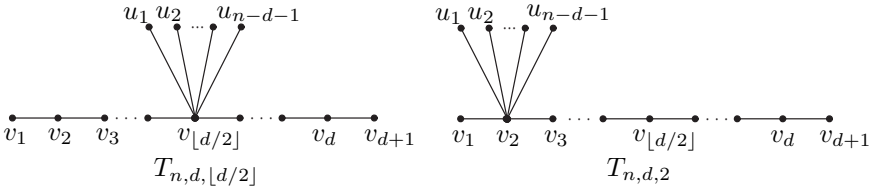

FIG. 1.1. *Graphs $T_{n,d,\lfloor d/2\rfloor}$ and $T_{n,d,2}$.*

An interesting fact is that among n-vertex trees with a given bipartition, the extremal one that minimizes the Laplacian permanent [1] is exactly the one that simultaneously minimizes all Laplacian coefficients; see [13]. Up to now, it is natural for us to find some interesting classes of graphs such that the extremal graphs which has smallest the Laplacian permanent and the Laplacian coefficients among these classes respectively are the same.

Motivated by [1, 13], in this paper, we use a new and unified method to show some known results on the Laplacian permanent, as well we use the edge-grafting transformations to identify the n-vertex trees of given bipartition having the second and third smallest Laplacian permanent. Similarly, we also characterize the n-vertex bipartite unicyclic graphs of given bipartition having the first, second and third smallest Laplacian permanent. Consequently, we identify the n-vertex bipartite unicyclic graphs with the first, second and third smallest Laplacian permanent.

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2. Three edge-grafting theorems on Laplacian permanent. In this section, we introduce three edge grafting transformations and study their properties.

DEFINITION 2.1. Let uv be a pendant edge of an n-vertex bipartite graph G with $d(u) = 1$, $n \geq 3$. Let $w\,(\neq v)$ be a vertex of G with $d(w) \geq d(v)$. Let $G[v \to w; 1]$ be the graph obtained from G by deleting the edge uv and adding the edge uw. In notation,

$$G[v \to w; 1] = G - uv + uw$$

and we say $G[v \to w; 1]$ is obtained from G by *Operation I.*

THEOREM 2.2. *Let G and $G[v \to w; 1]$ be the bipartite graphs defined as above. Then* $\mathrm{per}L(G) > \mathrm{per}L(G[v \to w; 1])$.

Proof. Let $d_G(v) = r$ and $d_G(w) = t$. First we consider that $vw \notin E_G$. With an appropriate ordering of the vertices of G and $G[v \to w; 1]$ as $u, v, w, \ldots$, we see that

$$L(G) = \begin{pmatrix} 1 & -1 & 0 & \mathbf{0} \\ -1 & r & 0 & \mathbf{x}_1 \\ 0 & 0 & t & \mathbf{x}_2 \\ \mathbf{0} & \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{A} \end{pmatrix}$$

and

$$L(G[v \to w; 1]) = \begin{pmatrix} 1 & 0 & -1 & \mathbf{0} \\ 0 & r-1 & 0 & \mathbf{x}_1 \\ -1 & 0 & t+1 & \mathbf{x}_2 \\ \mathbf{0} & \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{A} \end{pmatrix}.$$

Let M_1 (resp., M_2) be the matrix obtained from $L(G)$ (resp., $L(G[v \to w; 1])$) by eliminating the first row and the first column. Let N_1 (resp., N_2) be the matrix obtained from $L(G)$ (resp., $L(G[v \to w; 1])$) by eliminating the first 2 rows and the first 2 columns. And let N_2' be the matrix obtained from M_2 by eliminating its second row and second column. Then we have

$$\mathrm{per}L(G) = \mathrm{per}M_1 + \mathrm{per}N_1, \quad \mathrm{per}L(G[v \to w; 1]) = \mathrm{per}M_2 + \mathrm{per}N_2'.$$

Set

$$S_1 = \mathrm{per}\begin{pmatrix} 0 & \mathbf{x}_2 \\ \mathbf{y}_2 & \mathbf{A} \end{pmatrix}, \qquad S_2 = \mathrm{per}\begin{pmatrix} 0 & \mathbf{x}_1 \\ \mathbf{y}_1 & \mathbf{A} \end{pmatrix}.$$

Note that

$$\mathrm{per}N_1 = t \cdot \mathrm{per}A + S_1, \quad \mathrm{per}N_2' = (r-1) \cdot \mathrm{per}A + S_2, \quad \mathrm{per}M_2 = \mathrm{per}M_1 + \mathrm{per}N_2' - \mathrm{per}N_1.$$

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Hence,

$$\text{per}L(G) - \text{per}L(G[v \to w; 1]) = 2((t-r)\cdot \text{per}A + \text{per}A + S_1 - S_2). \tag{2.1}$$

By the choice of S_1 and S_2, we have

$$\text{per}A + S_1 > S_2. \tag{2.2}$$

Note that $t \geq r$, by (2.1) and (2.2) we get $\text{per}L(G) - \text{per}L(G[v \to w; 1]) > 0$.

Now consider $vw \in E_G$. By a similar argument as in the proof of the case $vw \notin E_G$, we can also get $\text{per}L(G) - \text{per}L(G[v \to w; 1]) > 0$. We omit the procedure here. □

DEFINITION 2.3. Let vw be an edge of a bipartite graph U with $d(w) \geq 2$. G is obtained from U and the star S_{k+2} by identifying v with a pendant vertex of S_{k+2} whose center is u. Let $G[u \to w; 2]$ be the graph obtained from G by deleting all edges $uz, z \in W$ and adding all edges $wz, z \in W$, where $W = N_G(u)\backslash\{v\}$. In notation,

$$G[u \to w; 2] = G - \{uz : z \in W\} + \{wz : z \in W\}$$

and we say $G[u \to w; 2]$ is obtained from G by *Operation II*. Graphs G and $G[u \to w; 2]$ are depicted in Fig. 2.1.

FIG. 2.1. *$G \Rightarrow G[u \to w; 2]$ by Operation II.*

THEOREM 2.4. *Let G and $G[u \to w; 2]$ be the bipartite graphs described as above. Then* $\text{per}L(G) > \text{per}L(G[u \to w; 2])$.

Proof. Let $N_G(u)\backslash\{v\} = \{u_1, u_2, \ldots, u_k\}$, where $k \geq 1$, $u_1, u_2, \ldots, u_k$ are pendant vertices. With an appropriate ordering of the vertices of G and $G[u \to w; 2]$ as $u_1, u_2, \ldots, u_k, u, v, w, \ldots$, we have

$$L(G) = \left(\begin{array}{ccc|c|ccc} 1 & & & -1 & & & \\ & \ddots & & \vdots & & & \\ & & 1 & -1 & & & \\ \hline -1 & \cdots & -1 & k+1 & -1 & & \\ \hline & & & -1 & d_v & -1 & \mathbf{x}_1 \\ & & & & -1 & d_w & \mathbf{x}_2 \\ & & & & \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{A} \end{array}\right)$$

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and

$$L(G[u\to w;2]) = \left(\begin{array}{ccc|cc|cc} 1 & & & & & -1 & \\ & \ddots & & & & \vdots & \\ & & 1 & & & -1 & \\ \hline & & & 1 & -1 & 0 & \\ & & & -1 & d_v & -1 & \mathbf{x}_1 \\ \hline -1 & \cdots & -1 & 0 & -1 & d_w+k & \mathbf{x}_2 \\ & & & & \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{A} \end{array}\right),$$

where d_v and d_w are degrees of v and w in G with $d_w \geq 2$.

Let D_1 (resp., D_2) be the matrix obtained from $L(G)$ (resp., $L(G[u\to w;2])$) by eliminating the first $k+1$ rows and the first $k+1$ columns; let M_1 (resp., M_2) be the matrix obtained from D_1 (resp., D_2) by eliminating the first row and the first column. Let M be the matrix obtained from D_1 by eliminating the second row and the second column, and let $M(i)$ (resp., $N(i)$) $(1 \leq i \leq k)$ be the matrix obtained from $L(G[u\to w;2])$ by eliminating the rows and columns corresponding to $u_1, u_2, \ldots, u_{k-i}$ and u (resp., $u_1, u_2, \ldots, u_{k-i}, u$ and v).

It is routine to check that $\{\mathrm{per}M(i), 1 \leq i \leq k\}$ and $\{\mathrm{per}N(i), 1 \leq i \leq k\}$, respectively, have the recurrence relation

$$\mathrm{per}M(i) = \mathrm{per}M(i-1) + \mathrm{per}M, \quad \mathrm{per}N(i) = \mathrm{per}N(i-1) + \mathrm{per}A, \quad 2 \leq i \leq k$$

with initial value $\mathrm{per}M(1) = \mathrm{per}D_2 + \mathrm{per}M$ and $\mathrm{per}N(1) = \mathrm{per}M_2 + \mathrm{per}A$. Hence,

$$\mathrm{per}M(k) = \mathrm{per}D_2 + k\cdot\mathrm{per}M, \quad \mathrm{per}N(k) = \mathrm{per}M_2 + k\cdot\mathrm{per}A. \tag{2.3}$$

By expanding the permanent of $L(G)$ along the first $(k+1)$ rows we obtain

$$\mathrm{per}L(G) = (2k+1)\cdot\mathrm{per}D_1 + \mathrm{per}M_1, \tag{2.4}$$

and by expanding the permanent of $L(G[u\to w;2])$ along the row corresponding to u, we get

$$\mathrm{per}L(G[u\to w;2]) = \mathrm{per}M(k) + \mathrm{per}N(k).$$

Note that $\mathrm{per}D_2 = \mathrm{per}D_1 + k\cdot\mathrm{per}M$ and $\mathrm{per}M_2 = \mathrm{per}M_1 + k\cdot\mathrm{per}A$. Hence, by (2.3)

$$\mathrm{per}L(G[u\to w;2]) = \mathrm{per}D_1 + 2k\cdot\mathrm{per}M + \mathrm{per}M_1 + 2k\cdot\mathrm{per}A. \tag{2.5}$$

For convenience, denote by D_1' the matrix obtained from D_1 by replacing d_w with

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$d_w - 1$. In view of (2.4) and (2.5), we get

$$\begin{aligned}\mathrm{per}L(G) - \mathrm{per}L(G[u \to w; 2]) &= 2k \cdot \mathrm{per}D_1 - 2k \cdot \mathrm{per}M - 2k \cdot \mathrm{per}A \\ &= 2k(\mathrm{per}D_1' + \mathrm{per}M) - 2k \cdot \mathrm{per}M - 2k \cdot \mathrm{per}A \\ &= 2k(\mathrm{per}D_1' - \mathrm{per}A) \\ &\geq 2k[(d_v(d_w - 1) + 1) \cdot \mathrm{per}A - \mathrm{per}A] \\ &> 0. \quad \square\end{aligned}$$

DEFINITION 2.5. Let G be an n-vertex graph obtained from $C_{2k} = v_1v_2 \cdots v_i \cdots v_j \cdots v_{2k}v_1$ $(k \geq 3)$ and two stars S_{n_i+1}, S_{n_j+1} by identifying v_i (resp., v_j) with the center of S_{n_i+1} (resp., S_{n_j+1}), where $4 < i < j$, $n = 2k + n_i + n_j$; see Fig. 2.2. Let $G' = G - v_1v_2 + v_1v_4$. Then we say that G' is obtained from G by *Operation III*.

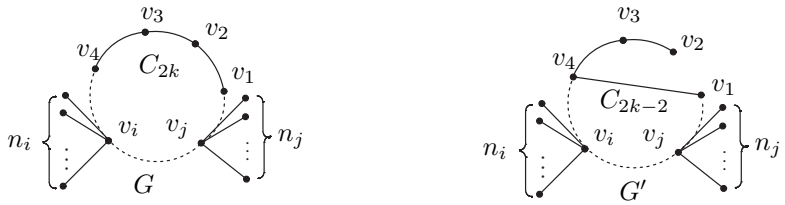

FIG. 2.2. $G \Rightarrow G'$ *by Operation III.*

THEOREM 2.6. *Let G and G' be the bipartite unicyclic graphs described as above. Then* $\mathrm{per}L(G) > \mathrm{per}L(G')$.

Proof. Ordering the vertices of G as $v_1, v_2, v_3, v_4, \ldots$, we have

$$L(G) = \begin{pmatrix} 2 & -1 & & & \mathbf{x}_1 \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & \mathbf{x}_4 \\ \mathbf{y}_1 & & & \mathbf{y}_4 & \mathbf{A} \end{pmatrix}.$$

Ordering the vertices of G' as $v_2, v_3, v_4, v_1, \ldots$, we see that

$$L(G') = \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 3 & -1 & \mathbf{x}_4 \\ & & -1 & 2 & \mathbf{x}_1 \\ & & \mathbf{y}_4 & \mathbf{y}_1 & \mathbf{A} \end{pmatrix}.$$

Let D (resp., D') be the matrix obtained from $L(G)$ (resp., $L(G')$) by eliminating the rows and columns corresponding to v_2 and v_3; and let M_1 (resp., M_2) be obtained

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from $L(G)$ (resp., $L(G')$) by eliminating rows and columns corresponding to v_2, v_3, v_4 (resp., v_1, v_2, v_3). And for convenience, denote

$$N_1 = \begin{pmatrix} 0 & \mathbf{x}_1 \\ \mathbf{y}_4 & \mathbf{A} \end{pmatrix}, \qquad N_2 = \begin{pmatrix} 0 & \mathbf{x}_4 \\ \mathbf{y}_1 & \mathbf{A} \end{pmatrix}.$$

Expanding the rows corresponding to v_2 and v_3 of $L(G)$ and $L(G')$, respectively, yields

$$\begin{aligned} \mathrm{per}L(G) &= -\mathrm{per}N_1 + 2\mathrm{per}M_2 + \mathrm{per}A + 5\mathrm{per}D + 2\mathrm{per}M_1 - \mathrm{per}N_2, \\ \mathrm{per}L(G') &= 3\mathrm{per}D' + \mathrm{per}M_1. \end{aligned}$$

Together with $\mathrm{per}D' = \mathrm{per}D + \mathrm{per}M_1 + \mathrm{per}A - \mathrm{per}N_1 + \mathrm{per}N_2$, we obtain

$$\mathrm{per}L(G') = 3\mathrm{per}D + 4\mathrm{per}M_1 + 3\mathrm{per}A - 3\mathrm{per}N_1 - 3\mathrm{per}N_2$$

and hence

$$\begin{aligned} \mathrm{per}L(G) - \mathrm{per}L(G') =& 2\mathrm{per}D + 2\mathrm{per}M_2 + 2\mathrm{per}N_1 + 2\mathrm{per}N_2 - 2\mathrm{per}M_1 - 2\mathrm{per}A \\ =& 2(\mathrm{per}D - \mathrm{per}M_1) + 2(\mathrm{per}M_2 - \mathrm{per}A) + 2\mathrm{per}N_1 + 2\mathrm{per}N_2. \end{aligned} \tag{2.6}$$

By ordering the vertices of G as $v_1, v_2, v_3, v_4, \ldots, v_i, \ldots, v_j, \ldots, v_{2k}, \ldots$, and by direct calculation, we have $\mathrm{per}N_1 = \mathrm{per}N_2 = -1$. And note that

$$(\mathrm{per}D - \mathrm{per}M_1) + (\mathrm{per}M_2 - \mathrm{per}A) = \mathrm{per}\begin{pmatrix} 3 & 0 & \mathbf{x}_1 \\ 0 & 1 & \mathbf{x}_4 \\ \mathbf{y}_1 & \mathbf{y}_4 & \mathbf{A} \end{pmatrix} \geq 3.$$

Together with (2.6), we have

$$\mathrm{per}L(G) - \mathrm{per}L(G') \geq 2 \times 3 + 2(-1) + 2(-1) = 2 > 0. \quad \square$$

3. Applications.

3.1. Laplacian permanents of trees among $\mathscr{T}_n^{p,q}$. We denote by $D(p,q)$ a *double star* with n vertices, which is obtained from an edge vw by attaching $p-1$ (resp., $q-1$) pendant vertices to v (resp., w), where $n = p+q$. Let $D'(p-1,q-1)$ (resp., $D''(p-1,q-1)$) be an n-vertex tree obtained from $D(p-1,q-1)$ by attaching a pendant path of length 2 to w (resp., v). Graphs $D(p,q)$, $D'(p-1,q-1)$, $D''(p-1,q-1)$ are depicted in Fig. 3.1. Let $T(n,k,a)$ be an n-vertex tree obtained by attaching a and $n-k-a$ pendant vertices to the two end-vertices of P_k, respectively. In particular, $D(p,q) = T(n,2,p-1)$.

The following lemma is routine to check.

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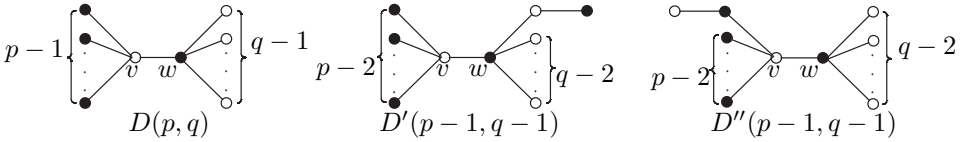

FIG. 3.1. *Trees $D(p,q), D'(p-1,q-1)$ and $D''(p-1,q-1)$.*

LEMMA 3.1. *Let p and q be positive integers, then*

$$\mathrm{per}L(D'(p-1,q-1)) = (2p-3)(6q-5)+3,\ \mathrm{per}L(D''(p-1,q-1)) = (2q-3)(6p-5)+3.$$

From Lemma 3.1, a direct calculation yields

$$\mathrm{per}L(D'(p-1,q-1)) < \mathrm{per}L(D''(p-1,q-1)) \qquad \text{for } q > p > 2. \tag{3.1}$$

From [1] we know that $D(p,q)$ minimizes the Laplacian permanent of trees among $\mathscr{T}_n^{p,q}$. In this subsection, we use a new and unified method to determine the tree in $\mathscr{T}_n^{p,q}$ which has the first, second, and third smallest Laplacian permanent, respectively.

THEOREM 3.2 ([1]). *Let T be a tree with a (p, q)-bipartition. Then*

$$\mathrm{per}L(T) \geq (2p-1)(2q-1)+1$$

with equality if and only if T is a double-star $D(p,q)$.

Proof. Choose a tree T with a (p,q)-bipartition such that its Laplacian permanent is as small as possible. Let V_1, V_2 be the bipartition of the vertices of T with $V_1 = \{v_0, v_1, \ldots, v_{p-1}\}$, $V_2 = \{u_0, u_1, \ldots, u_{q-1}\}$. For convenience, let v_0 (resp., u_0) be the vertex of maximal degree among V_1 (resp., V_2) in T and let $A = N_T(v_0) \cap PV(T)$.

Hence, in order to complete the proof, it suffices to show the following claims.

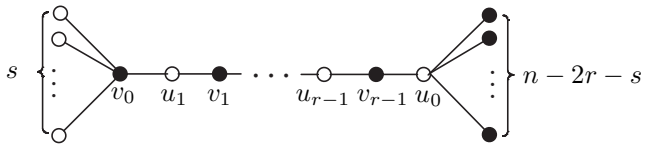

FIG. 3.2. *Tree $T(n, 2r, s)$ with some labelled vertices.*

CLAIM 1. *$T \cong T(n, 2r, s)$ (see Fig. 3.2) with $r \geq 1$ and $s \geq 0$.*

Proof of Claim 1. Otherwise, T must contain a pendant vertex $w \notin N_T(u_0) \cup N_T(v_0)$. Without loss of generality, we may assume $w \in V_2$ and its unique neighbor is

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w'. Using Operation I, let $T_0 = T - ww' + wv_0$. By Theorem 2.2 we have per$L(T_0) <$ per$L(T)$, a contradiction to the choice of T. ∎

Claim 2. *In the tree described as above, u_0 is adjacent to v_0.*

Proof of Claim 2. If not, then $d(u_0, v_0) \geq 3$. Note that v_0 is the maximal degree vertex among V_1, hence $d_T(v_0) \neq 1$, which implies $A \neq \emptyset$. Using Operation II, let

$$T_1 = T - \{v_0 z : z \in A\} + \{v_1 z : z \in A\}$$

then per$L(T_1) <$ per$L(T)$ by Theorem 2.4, which contradicts the choice of T. ∎

By Claims 1 and 2, we get that $T \cong D(p, q)$. By direct computing, we have

$$\text{per}L(D(p,q)) = (2p-1)(2q-1) + 1. \quad \square$$

Theorem 3.3. *Among $\mathscr{T}_n^{p,q}$.*

(i) *If $p = 2$, then all the members in $\mathscr{T}_n^{2,n-2}$ are ordered as follows:*

$$\text{per}L(D(2,n-2)) = \text{per}L(T(n,3,0)) < \text{per}L(T(n,3,1)) < \text{per}L(T(n,3,2)$$
$$< \cdots < \text{per}L(T(n,3,i)) < \cdots < \text{per}L\left(T\left(n,3,\left\lfloor\frac{n-3}{2}\right\rfloor\right)\right).$$

(ii) *If $p > 2$,*

(a) *for $T \in \mathscr{T}_n^{p,q} \setminus \{D(p,q)\}$, we have* per$L(T) \geq (2p-3)(6q-5)+3$. *The equality holds if and only if $T \cong D'(p-1, q-1)$.*

(b) *for $T \in \mathscr{T}_n^{p,q} \setminus \{D(p,q), D'(p-1,q-1)\}$ with $q > p$, we have* per$L(T) \geq (2q-3)(6p-5)+3$. *The equality holds if and only if $T \cong D''(p-1, q-1)$.*

Proof. (i) If $p = 2$, then

$$\mathscr{T}_n^{2,n-2} = \left\{T(n,3,0), T(n,3,1), \ldots, T(n,3,i), \ldots, T\left(n,3,\left\lfloor\frac{n-3}{2}\right\rfloor\right)\right\}.$$

By a simple calculation, we get

$$\text{per}L(T(n,3,i)) = -8\left(i - \frac{n-3}{2}\right)^2 + 2(n-3)^2 + 6n - 14.$$

Consider the function $f(x) = -8(x - \frac{n-3}{2})^2 + 2(n-3)^2 + 6n - 14$ in x with $0 \leq x \leq \lfloor\frac{n-3}{2}\rfloor$. By the monotonicity of $f(x)$, we have

$$f(0) < f(1) < \cdots < f(i-1) < f(i) < f(i+1) < \cdots < f\left(\left\lfloor\frac{n-3}{2}\right\rfloor\right). \tag{3.2}$$

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Note that $T(n,3,0) \cong D(2,n-2)$, together with (3.2) we get that (i) holds.

(ii) Choose $T \in \mathscr{T}_n^{p,q} \setminus \{D(p,q)\}$ such that its Laplacian permanent is as small as possible. Let V_1, V_2 be the bipartition of the vertices of T with $V_1 = \{v_0, v_1, \ldots, v_{p-1}\}$, $V_2 = \{u_0, u_1, \ldots, u_{q-1}\}$. For convenience, let v_0 (resp., u_0) be the vertex of maximal degree among V_1 (resp., V_2) in T and let $A = N_T(v_0) \cap PV(T)$. In order to complete the proof, it suffices to show the following claims.

Claim 1. $u_0v_0 \in E_T$.

Proof of Claim 1. If not, then $d_T(u_0, v_0) \geq 3$. In this case, we are to show that $T \cong T(n, 2r, s)$ (see Fig. 3.2). Otherwise, T must contain a pendant vertex $w \notin N_T(u_0) \cup N_T(v_0)$. Assume that the unique neighbor of w is w'. Using Operation I, let $T' = T - ww' + wv_0$ if $w \in V_2$ and $T' = T - ww' + wu_0$ otherwise. Note that $T' \in \mathscr{T}_n^{p,q} \setminus \{D(p,q)\}$, by Theorem 2.2 we have $\mathrm{per}L(T') < \mathrm{per}L(T)$, a contradiction to the choice of T. Hence, $T \cong T(n, 2r, s)$. On the one hand, $d_T(u_0, v_0) \geq 3$, hence $r \geq 2$; on the other hand, v_0 is of the maximal degree vertex in V_1 of T, hence $s \geq 1$. Therefore, $A \neq \emptyset$. Using Operation II, let

$$T_0 = T - \{v_0z : z \in A\} + \{v_1z : z \in A\}.$$

We also have $T_0 \in \mathscr{T}_n^{p,q} \setminus \{D(p,q)\}$. In view of Theorem 2.4, $\mathrm{per}L(T_0) < \mathrm{per}L(T)$, which also contradicts the choice of T. ∎

Claim 2. *In the tree T described as above, there exists a pendant vertex, say w, in V_T such that $d_T(w, u_0) = 2, d_T(w, v_0) = 3$ or $d_T(w, v_0) = 2, d_T(w, u_0) = 3$. Furthermore, for all $v \in PV(T) \setminus \{w\}$, v is adjacent to either u_0 or v_0.*

Proof of Claim 2. Note that $T \ncong D(p,q)$, hence there must exist a vertex (not necessarily a pendant vertex), say w, such that $d_T(w, u_0) = 2, d_T(w, v_0) = 3$ or $d_T(w, v_0) = 2, d_T(w, u_0) = 3$. With loss of generality, we assume that $d_T(w, u_0) = 2, d_T(w, v_0) = 3$. If w is not a pendant vertex, then w is on a path which joins u_0 and a pendant vertex, say r. Denote the unique neighbor of r by r'. Let $T' = T - rr' + ru_0$ if $r \in V_1$ and $T' = T - rr' + rv_0$ otherwise. It is routine to check that $T' \in \mathscr{T}_n^{p,q} \setminus \{D(p,q)\}$. By Theorem 2.2, $\mathrm{per}L(T') < \mathrm{per}L(T)$, a contradiction to the choice of T. Hence, w must be a pendant vertex.

In what follows, we show that for all $v \in PV(T) \setminus \{w\}$, either $vu_0 \in E_T$ or $vv_0 \in E_T$. In fact, if there exist a vertex, say y, in $PV(T) \setminus \{w\}$ such that $yu_0, yv_0 \notin E_T$. Denote the unique neighbor of y by y'. Let $\hat{T} = T - yy' + yu_0$ if $y \in V_1$ and $\hat{T} = T - yy' + yv_0$ otherwise. It is straightforward to check that $\hat{T} \in \mathscr{T}_n^{p,q} \setminus \{D(p,q)\}$. By Theorem 2.2, $\mathrm{per}L(\hat{T}) < \mathrm{per}L(T)$, a contradiction to the choice of T. ∎

By Claims 1 and 2, we obtain $T \cong D'(p-1, q-1)$, or $T \cong D''(p-1, q-1)$. If $p = q$, then $D'(p-1, q-1) \cong D''(p-1, q-1)$. Together with Lemma 3.1, (ii) holds

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obviously in this case. If $p < q$, then combining with Lemma 3.1 and Inequality (3.1), (ii) follows immediately. □

REMARK 3.4. We know from [13] that $D(p,q) \prec D'(p-1,q-1) \prec T$ for all $T \in \mathscr{T}_n^{p,q} \setminus \{D(p,q), D'(p-1,q-1)\}$. In view of Theorems 3.2 and 3.3, $D(p,q)$ (resp., $D'(p-1,q-1)$) is the tree with a (p,q) bipartition which has the smallest (resp., second smallest) Laplacian permanent. Hence, our result support the conjecture that trees minimizing the Laplacian permanent usually simultaneously minimize the Laplacian coefficients, and vice versa. Furthermore, in view of Theorems 3.2 and 3.3 it is natural to conjecture that $D(p,q) \prec D'(p-1,q-1) \prec D''(p-1,q-1) \prec T$ for all $T \in \mathscr{T}_n^{p,q} \setminus \{D(p,q), D'(p-1,q-1), D''(p-1,q-1)\}$ with $q > p$.

3.2. Laplacian permanent of trees with diameter at least d. Let Q_n be the matrix obtained from $L(P_{n+1})$ by eliminating row 1 and column 1. It is routine to check that $\mathrm{per}Q_1 = 1$ and $\mathrm{per}Q_2 = 3$. In particular, define $\mathrm{per}Q_0 = 1$. We know [1] that

$$\mathrm{per}Q_n = \frac{1}{2}(1+\sqrt{2})^n + \frac{1}{2}(1-\sqrt{2})^n \tag{3.3}$$

and

$$\mathrm{per}L(P_n) = \frac{2-\sqrt{2}}{2}(1+\sqrt{2})^n + \frac{2+\sqrt{2}}{2}(1-\sqrt{2})^n. \tag{3.4}$$

LEMMA 3.5 ([1]). *Let n, j and k be positive integers with $1 \le k < j \le \frac{1}{2}(n+1)$. Then $(-1)^k(\mathrm{per}Q_{j-1}\mathrm{per}Q_{n-j} - \mathrm{per}Q_{k-1}\mathrm{per}Q_{n-k}) > 0$.*

LEMMA 3.6 ([5]). *Let uv be the only non-pendant edge incidence with v in a tree T and let $A = N_T(v) \setminus \{u\}$. Let $T' = T - \{vz : z \in A\} + \{uz : z \in A\}$, then we have $\mathrm{per}L(T') < \mathrm{per}L(T)$.*

In this subsection, we use a new method to prove the following known result.

THEOREM 3.7 ([1]). *Let d be a positive integer, and let T be a tree with n vertices having diameter at least d. Then*

$$\mathrm{per}L(T) \ge \left(n-d+\frac{\sqrt{2}}{2}\right)(1+\sqrt{2})^{d-1} + \left(n-d-\frac{\sqrt{2}}{2}\right)(1-\sqrt{2})^{d-1}.$$

The equality holds if and only if $T \cong T_{n,d,2}$; see Fig. 1.1.

Proof. Choose an n-vertex tree T of diameter at least d such that its Laplacian permanent is as small as possible. If $T \cong P_{d+1}$, then our result holds by Theorem 1.1. Hence, in what follows we consider that $T \ncong P_{d+1}$. If T contains just two pendant

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vertices, i.e., $T \cong P_n = v_1v_2\cdots v_i\cdots v_n$. Let $T' = T - v_1v_2 + v_iv_1$. Obviously, T' is of diameter at least d. By Theorem 2.2, we have $\mathrm{per}L(T') < \mathrm{per}L(T)$, a contradiction to the choice of T. Hence, T contains at least 3 pendant vertices. That is to say, the maximal vertex degree in T is of at least 3. Without loss of generality, we may assume that w is just of the maximal degree vertex. Let $P' = v_1v_2\cdots v_i\cdots v_{l+1}$ be one of the longest paths contained in T, where $l \geq d$. In order to complete the proof, it suffices to show the following claims.

Claim 1. *$T \cong T_{n,l,i}$, where $T_{n,l,i}$ is obtained from P' by inserting $n-l-1$ pendant vertices at v_i, $i \in \{2,3,\ldots,\lfloor (l+2)/2\rfloor\}$.*

Proof of Claim 1. First we show that all the pendant vertices excluding the end-vertices of P' are adjacent to w. Assume to the contrary that $v \in PV(T)\setminus\{v_1, v_{l+1}\}$ satisfying $vw \notin E_T$. Denote the unique neighbor of v by v'. Set $T' = T - vv' + wv$. It is straightforward to check that T' is of an n-vertex tree of diameter at least d. By Theorem 2.2, we have $\mathrm{per}L(T') < \mathrm{per}L(T)$, a contradiction to the choice of T.

Now we show that w is on the path P'. Assume that w is not on the path P', then T must be the tree obtained by joining the center of a star S and a vertex of P' by a path of length at least 1. Denote the unique neighbor of w which is not a pendant vertex by w'. Set $A = N_T(w)\setminus\{w'\}$. Let $T' = T - \{wz : z \in A\} + \{w'z : z \in A\}$. It is easy to see that T' is a tree of diameter at least d. By Lemma 3.6, $\mathrm{per}L(T') < \mathrm{per}L(T)$, a contradiction. ∎

Claim 2. *In the tree $T_{n,l,i}$ described as above, we have $l = d, i = 2$, i.e., $T_{n,l,i} \cong T_{n,d,2}$.*

Proof of Claim 2. If not, then $l \geq d+1$. In the tree described above, let $T_2 = T_{n,l,i} - v_{l+1}v_l + v_iv_{l+1}$. It is easy to see that T_2 is an n-vertex tree of diameter at least d. By Theorem 2.2, we have $\mathrm{per}L(T_2) < \mathrm{per}L(T_{n,l,i})$, a contradiction to the choice of $T_{n,l,i}$. So we obtain $T \cong T_{n,d,i}$.

Expanding the permanent of $L(T_{n,d,i})$ along the row corresponding to vertex v_i gives

$$\mathrm{per}L(T_{n,d,i}) = \mathrm{per}L(P_{d+1}) + 2(n-d-1)\mathrm{per}Q_{i-1}\mathrm{per}Q_{d-i+1}.$$

This gives

$$\begin{aligned}\mathrm{per}L(T_{n,d,j}) - \mathrm{per}L(T_{n,d,2}) &= 2(n-d-1)(\mathrm{per}Q_{j-1}\mathrm{per}Q_{d-j+1} - \mathrm{per}Q_{2-1}\mathrm{per}Q_{d-2+1})\\ &> 0\end{aligned}$$

for $j = 3,4,\ldots,\lfloor \frac{1}{2}(d+2)\rfloor$, and the last inequality follows by Lemma 3.5. ∎

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In view of (3.3) and (3.4), we have

$$\text{per}L(T_{n,d,2}) = \left(n-d+\frac{\sqrt{2}}{2}\right)(1+\sqrt{2})^{d-1} + \left(n-d-\frac{\sqrt{2}}{2}\right)(1-\sqrt{2})^{d-1}. \tag{3.5}$$

By Claims 1 and 2, and Eq. (3.5), Theorem 3.7 follows immediately. □

3.3. Lower bounds for the Laplacian permanent of graphs in $\mathscr{U}_n^{p,q}$. In this subsection, we are to determine sharp lower bounds for the Laplacian permanent of graphs in $\mathscr{U}_n^{p,q}$. Let $C_4(1^{s_1}k_1, 1^{s_2}k_2, 1^{s_3}k_3, 1^{s_4}k_4)$ be the graph obtained from $C_4 = v_1v_2v_3v_4v_1$ by inserting s_i pendant vertices at v_i and joining v_i to the center of a star S_{k_i} by an edge, $i = 1, 2, 3, 4$; see Fig. 3.3. In particular, denote by $B(p, q) = C_4(1^{p-2}0, 1^{q-2}0, 1^00, 1^00)$.

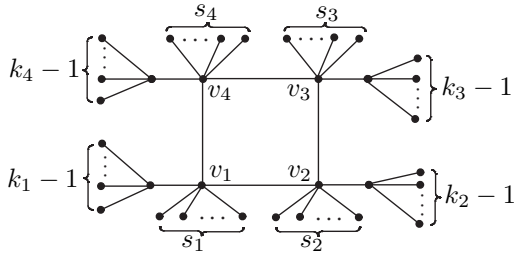

FIG. 3.3. *Graph* $C_4(1^{s_1}k_1, 1^{s_2}k_2, 1^{s_3}k_3, 1^{s_4}k_4)$.

THEOREM 3.8. *For any* $G \in \mathscr{U}_n^{p,q}$, *one has* $\text{per}L(G) \geq 20(p-1)(q-1)+4n$. *The equality holds if and only if* $G \cong B(p,q)$.

Proof. Choose $G \in \mathscr{U}_n^{p,q}$ such that its Laplacian permanent is as small as possible. If $n = 4, 5$, $\mathscr{U}_4^{p,q} = \{B(2,2)\}$ and $\mathscr{U}_5^{p,q} = \{B(2,3)\}$, our result holds obviously. Hence in what follows we consider $n \geq 6$. Let C_r be the unique cycle contained in G. Note that, by Theorem 2.6, $G \ncong C_n$. Hence, $PV(G) \neq \emptyset$. Let V_1, V_2 be the bipartition of V_G such that $|V_1| = p$ and $|V_2| = q$ with v_0 (resp., u_0) being of the maximal degree vertex among V_1 (resp., V_2) in G.

CLAIM 1. *For all* $u \in PV(G)$, *either* $uu_0 \in E_G$ *or* $uv_0 \in E_G$.

Proof of Claim 1. If not, then there exists a pendant vertex, say u, such that u is not in $N_G(u_0) \cup N_G(v_0)$. Denote the unique neighbor of u by u'. Using Operation I, let $G' = G - uu' + uu_0$ if $u \in V_1$ and $G' = G - uu' + uv_0$ otherwise. It is routine to check that $G' \in \mathscr{U}_n^{p,q}$. By Theorem 2.2, $\text{per}L(G') < \text{per}L(G)$, a contradiction to the choice of G. ■

Let $d(u, C_r) = \min\{d(u, v) : v \in V_{C_r}\}$. In particular, if u is on C_r, then $d(u, C_r) =$

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0.

CLAIM 2. $d(v_0, C_r) = d(u_0, C_r) = 0$.

Proof of Claim 2. Here we only show that $d(v_0, C_r) = 0$ by contradiction. With the same method, we can also show $d(u_0, C_r) = 0$.

Assume that $d(v_0, C_r) = t \geq 1$. Set $A = PV(G) \cap N_G(v_0)$. By Claim 1, we have $A \neq \emptyset$. Let $P_t = v_0 w_1 w_2 \cdots w_{t-1} w_t$ be the shortest path connecting v_0 and the cycle C_r, where w_t is on C_r. Let $u \in V_{C_r} \cap N_G(w_t)$. Using Operation II, let

$$\bar{G} = \begin{cases} G - \{zv_0 : z \in A\} + \{zu : z \in A\}, & \text{if } t = 1; \\ G - \{zv_0 : z \in A\} + \{zw_2 : z \in A\}, & \text{if } t \geq 2. \end{cases}$$

It is routine to check that $\bar{G} \in \mathscr{U}_n^{p,q}$. By Theorem 2.4, we have $\mathrm{per}L(\bar{G}) < \mathrm{per}L(G)$, a contradiction to the choice of G. ∎

CLAIM 3. $r \leq 6$.

Proof of Claim 3. If not, then $r \geq 8$. By the structure of G described as above, then there must exist four consecutive vertices, say $u_{k_1}, v_{k_1}, u_{k_2}, v_{k_2}$ on the cycle C_r such that $u_0, v_0 \notin \{u_{k_1}, v_{k_1}, u_{k_2}, v_{k_2}\}$. Without loss of generality assume that $v_{k_1}, v_{k_2} \in V_1$ and $u_{k_1}, u_{k_2} \in V_2$. Using Operation III, let $G_0 = G - u_{k_1}v_{k_1} + u_{k_1}v_{k_2}$. It is routine to check that $G_0 \in \mathscr{U}_n^{p,q}$. By Theorem 2.6 $\mathrm{per}L(G_0) < \mathrm{per}L(G)$, a contradiction to the choice of G. ∎

Hence, by Claims 1–3, we obtain

- $r = 4$, then $G \cong B(p, q)$.
- $r = 6$, then $G \cong G_1$ or G_2, where G_1, G_2 are depicted in Fig. 3.4.

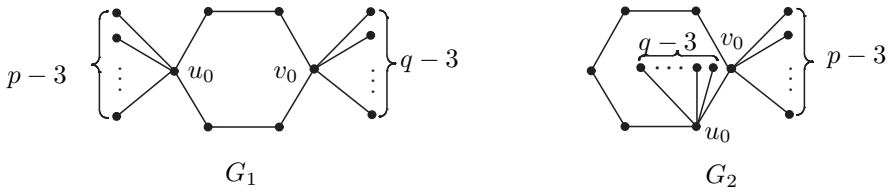

FIG. 3.4. *Graphs G_1 and G_2.*

If $G \cong G_2$, using Operation III on G_2, we obtain graph $C_4(1^0 2, 1^{q-3}0, 1^{p-3}0, 1^0 0)$ which is in $\mathscr{U}_n^{p,q}$. By Theorem 2.6, we have $\mathrm{per}L(C_4(1^0 2, 1^{q-3}0, 1^{p-3}0, 1^0 0)) < \mathrm{per}L(G)$, a contradiction to the choice of G. So $G \ncong G_2$.

If $G \cong G_1$, by a simple calculation, we get

$$\begin{aligned} \mathrm{per}L(G_1) &= 100(p-2)(q-2) + 40n - 140, \\ \mathrm{per}L(B(p,q)) &= 20(p-1)(q-1) + 4n. \end{aligned} \tag{3.6}$$

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Note that $p+q=n$ with $3 \le p \le q \le n-3$, hence

$$pq \ge 3(n-3). \tag{3.7}$$

Hence,

$$\begin{aligned} \mathrm{per}L(G_1) - \mathrm{per}L(B(p,q)) &= 80pq - 144n + 240 \\ &\ge 80 \cdot 3(n-3) - 144n + 240 \quad \text{(by (3.7))} \\ &= 96n - 480 \\ &> 0. \end{aligned}$$

Therefore, $\mathrm{per}L(G_1) > \mathrm{per}L(B(p,q))$. Thus, we obtain $G \cong B(p,q)$. Together with Eq. (3.6), we complete the proof. □

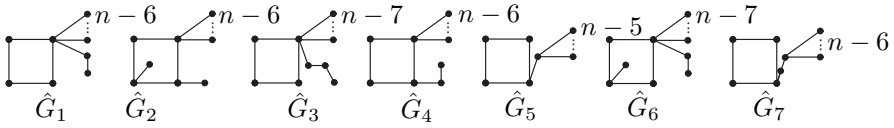

FIG. 3.5. *Graphs* $\hat{G}_1, \hat{G}_2, \ldots, \hat{G}_7$.

Next we are to identify the graph in $\mathscr{U}_n^{p,q}$ with the second (resp., third) smallest Laplacian permanent.

THEOREM 3.9. *Among* $\mathscr{U}_n^{p,q}$.

(i) *If* $p=2$, *the ordering of all the members in* $\mathscr{U}_n^{2,n-2}$ *with* $n \ge 4$ *is as follows:* $\mathrm{per}L(B(2,n-2)) < \mathrm{per}L(C_4(1^1 0, 1^0 0, 1^{n-5} 0, 1^0 0)) < \cdots < \mathrm{per}L(C_4(1^i 0, 1^0 0, 1^{n-4-i} 0, 1^0 0)) < \cdots < \mathrm{per}L(C_4(1^{\lfloor \frac{n-4}{2} \rfloor} 0, 1^0 0, 1^{\lceil \frac{n-4}{2} \rceil} 0, 1^0 0))$.

(ii) *If* $p=3$, *then* $\mathrm{per}L(B(3,n-3)) < \mathrm{per}L(\hat{G}_1) < \mathrm{per}L(\hat{G}_2) < \mathrm{per}L(G)$ *for all* $G \in \mathscr{U}_n^{3,n-3} \setminus \{B(3,n-3), \hat{G}_1, \hat{G}_2\}$ *with* $n \ge 20$, *where* $\hat{G}_1, \hat{G}_2$ *are depicted in Fig. 3.5.*

(iii) *If* $p \ge 4$,
   (a) *for all* $G \in \mathscr{U}_n^{p,q} \setminus \{B(p,q)\}$ *with* $n \ge 8$, *one has* $\mathrm{per}L(G) \ge 36(p-2)(q-1) + 4p + 8q - 4$ *with equality if and only if* $G \cong C_4(1^{q-2}0, 1^{p-3}0, 1^0 0, 1^1 0)$.

   (b) *for all* $G \in \mathscr{U}_n^{p,q} \setminus \{B(p,q), C_4(1^{q-2}0, 1^{p-3}0, 1^0 0, 1^1 0)\}$ *with* $q > p$, $n \ge 9$, *one has* $\mathrm{per}L(G) \ge 36(q-2)(p-1) + 4q + 8p - 4$ *with equality if and only if* $G \cong C_4(1^{q-3}0, 1^{p-2}0, 1^1 0, 1^0 0)$.

Proof. (i) If $p=2$, then

$$\mathscr{U}_n^{2,n-2} = \left\{ C_4(1^i 2^0, 1^0 2^0, 1^{n-4-i} 2^0, 1^0 2^0) : 0 \le i \le \left\lfloor \frac{n-4}{2} \right\rfloor \right\}.$$

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By a simple calculation, we get

$$\mathrm{per}L(C_4(1^i2^0,1^02^0,1^{n-4-i}2^0,1^02^0)) = -16\left(i-\frac{n-4}{2}\right)^2+4(n-1)^2.$$

Consider the function $f(x) = -16(x-\frac{n-4}{2})^2+4(n-1)^2$ in x with $0 \le x \le \lfloor \frac{n-4}{2} \rfloor$. By the monotonicity of $f(x)$, we have

$$f(0) < f(1) < \cdots < f(i) < \cdots < f\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right). \tag{3.8}$$

Note that $C_4(1^00,1^00,1^{n-4}0,1^00) \cong B(2,n-2)$, hence (i) follows immediately from (3.8).

(ii) Note that $p=3$, hence the cycle C_r contained in $T \in \mathscr{U}_n^{3,n-3}$ is of length at most 6, i.e., $r \le 6$. If $r=4$, the bipartite unicyclic graph, say U (resp., U'), in $\mathscr{U}_n^{3,n-3}$ with the second (resp., third) smallest Laplacian permanent should satisfy the following property: Apply Operation I (or II) to U (resp., U') only once to get the graph $B(3,n-3)$ (resp., $B(3,n-3)$ or U). Hence, $U,U' \in \{\hat{G}_1,\hat{G}_2,\hat{G}_3,\hat{G}_4,\hat{G}_5,\hat{G}_6,\hat{G}_7,\hat{G}_8\}$, where $\hat{G}_1,\hat{G}_2,\ldots,\hat{G}_8$ are depicted in Fig. 3.5.

If $r=6$, then graph G_1 (see Fig. 3.4) is the possible graph with the smallest Laplacian permanent. By direct calculation, we have

$$\begin{array}{lll}
\mathrm{per}L(\hat{G}_1) = 72n-276, & \mathrm{per}L(\hat{G}_2) = 76n-352, & \mathrm{per}L(\hat{G}_3) = 168n-804,\\
\mathrm{per}L(\hat{G}_4) = 112n-516, & \mathrm{per}L(\hat{G}_5) = 96n-420, & \mathrm{per}L(\hat{G}_6) = 120n-580,\\
\mathrm{per}L(\hat{G}_7) = 216n-1140, & \mathrm{per}L(G_1) = 140n-640. &
\end{array}$$

Based on the above direct computing, (ii) follows immediately.

(iii) We first determine the graph, say G, in $\mathscr{U}_n^{p,q}$ with the second smallest Laplacian permanent for $p \ge 4$. In view of the proof of Theorem 3.8, it is easy to see that the cycle C_r contained in G is of length at most 6. Furthermore, if $r=6$, only G_1 as depicted in Fig. 3.4 is possible to be the particular graph G. If $r=4$, in view of Theorems 2.2 and 2.4, we know that $B(p,q)$ can be obtained from G by Operation I (or, II) once. Hence, based on Operation I, G may be $C_4(1^{q-2}0,\ 1^{p-3}0,1^00,1^10)$ or $C_4(1^{q-3}0,1^{p-2}0,1^10,1^00)$; whereas based on Operation II, G may be in the set

$$\mathscr{A} = \{C_4(1^{q-3}(t+1),1^{p-2-t}0,1^00,1^00) : 1 \le t \le p-2\}$$

or

$$\mathscr{B} = \{C_4(1^{q-2-t}0,1^{p-3}(t+1),1^00,1^00) : 1 \le t \le q-2\}.$$

Combining with Operation I we see that $\mathscr{A}$ (resp., $\mathscr{B}$) contains just two members $C_4(1^{q-3}2,1^{p-3}0,1^00,1^00)$ and $C_4(1^{q-3}(p-1),1^00,1^00,1^00)$ (resp., $C_4(1^{q-3}0,1^{p-3}2,$

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$1^0 0, 1^0 0)$ and $C_4(1^0 0, 1^{p-3}(q-1), 1^0 0, 1^0 0))$. Hence, summarizing the discussion as above we get that G must be in $\mathscr{U}' = \{C_4(1^{q-2}0, 1^{p-3}0, 1^0 0, 1^1 0), C_4(1^{q-3}0, 1^{p-2}0, 1^1 0, 1^0 0), C_4(1^{q-3}2, 1^{p-3}0, 1^0 0, 1^0 0), C_4(1^{q-3}0, 1^{p-3}2, 1^0 0, 1^0 0), C_4(1^0 0, 1^{p-3}(q-1), 1^0 0, 1^0 0), C_4(1^{q-3}(p-1), 1^0 0, 1^0 0, 1^0 0), G_1\}$.

By direct calculation, we obtain

$$\begin{aligned}
\mathrm{per}L(C_4(1^{q-2}0, 1^{p-3}0, 1^0 0, 1^1 0)) &= 36pq - 32n - 32q + 68,\\
\mathrm{per}L(C_4(1^{q-3}0, 1^{p-2}0, 1^1 0, 1^0 0)) &= 36pq - 32n - 32p + 68,\\
\mathrm{per}L(C_4(1^{q-3}2, 1^{p-3}0, 1^0 0, 1^0 0)) &= 60pq - 68n - 40q + 144,\\
\mathrm{per}L(C_4(1^{q-3}0, 1^{p-3}2, 1^0 0, 1^0 0)) &= 60pq - 68n - 40p + 144,\\
\mathrm{per}L(C_4(1^{q-3}(p-1), 1^0 0, 1^0 0, 1^0 0)) &= 48pq - 72n + 24p + 84,\\
\mathrm{per}L(C_4(1^0 0, 1^{p-3}(q-1), 1^0 0, 1^0 0)) &= 48pq - 72n + 24q + 84.
\end{aligned}$$

This gives

(3.9)
$$\mathrm{per}L(C_4(1^{q-2}0, 1^{p-3}0, 1^0 0, 1^1 0)) < \mathrm{per}L(C_4(1^{q-3}0, 1^{p-2}0, 1^1 0, 1^0 0)) < \mathrm{per}L(\hat{G})$$

for all $\hat{G} \in \mathscr{U}' \setminus \{C_4(1^{q-2}0, 1^{p-3}0, 1^0 0, 1^1 0), C_4(1^{q-3}0, 1^{p-2}0, 1^1 0, 1^0 0)\}$ for $q > p \geq 4$. This completes the proof of the first part of (iii).

Now we show the second part of (iii). By a similar discussion as in the proof of the first part of (iii), we know that the graph, say G', in $\mathscr{U}_n^{p,q}$ having the third smallest Laplacian permanent is either the graph with the second smallest Laplacian permanent in $\mathscr{U}'$, or apply Operation I (or II) once to G' to obtain the graph $C_4(1^{q-2}0, 1^{p-3}0, 1^0 0, 1^1 0)$, which has the second smallest Laplacian permanent in $\mathscr{U}_n^{p,q}$. Hence, together with (3.9), we obtain that G' is in the set $\mathscr{U}'' = \{C_4(1^{q-3}0, 1^{p-2}0, 1^1 0, 1^0 0), C_4(1^{q-3}2, 1^{p-3}0, 1^0 0, 1^0 0), C_4(1^{q-3}0, 1^{p-4}2, 1^0 0, 1^1 0), C_4(1^{q-3}2, 1^{p-4}0, 1^0 0, 1^1 0), C_4(1^{q-3}0, 1^{p-3}0, 1^0 0, 1^0 2), C_4(1^{q-3}0, 1^{p-3}0, 1^1 0, 1^1 0), C_4(1^0 0, 1^{p-4}(q-1), 1^0 0, 1^1 0), C_4(1^{q-3}(p-2), 1^0 0, 1^0 0, 1^1 0), C_4(1^0 0, 1^{p-3}0, 1^0 0, 1^0(q-1))\}$.

By direct calculation, we have

$$\begin{aligned}
\mathrm{per}L(C_4(1^{q-3}2, 1^{p-3}0, 1^0 0, 1^0 0)) &= 60pq - 68n - 40q + 144,\\
\mathrm{per}L(C_4(1^{q-3}0, 1^{p-4}2, 1^0 0, 1^1 0)) &= 108pq - 24q - 204n + 464,\\
\mathrm{per}L(C_4(1^{q-3}2, 1^{p-4}0, 1^0 0, 1^1 0)) &= 108pq - 168q - 132n + 400,\\
\mathrm{per}L(C_4(1^{q-3}0, 1^{p-3}0, 1^0 0, 1^0 2)) &= 92pq + 8q - 172n + 336,\\
\mathrm{per}L(C_4(1^{q-3}0, 1^{p-3}0, 1^1 0, 1^1 0)) &= 68pq - 128n + 260,\\
\mathrm{per}L(C_4(1^0 0, 1^{p-4}(q-1), 1^0 0, 1^1 0)) &= 80pq - 40q - 120n + 260,\\
\mathrm{per}L(C_4(1^{q-3}(p-2), 1^0 0, 1^0 0, 1^1 0)) &= 88pq - 120q - 100n + 272,\\
\mathrm{per}L(C_4(1^0 0, 1^{p-3}0, 1^0 0, 1^0(q-1))) &= 64pq + 8p - 96n + 132.
\end{aligned}$$

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Based on the above direct computing, the second part of (iii) follows immediately. □

REMARK 3.10. In view of Theorems 3.8 and 3.9, we hope to show that, among the set of all n-vertex unicyclic graphs with a (p,q)-bipartition($q > p \geq 4$), $B(p,q) \prec C_4(1^{q-2}0, 1^{p-3}0, 1^00, 1^10) \prec C_4(1^{q-3}0, 1^{p-2}0, 1^10, 1^00) \prec G$ for all $G \in \mathscr{U}_n^{p,q} \setminus \{B(p,q), C_4(1^{q-2}0, 1^{p-3}0, 1^00, 1^10), C_4(1^{q-3}0, 1^{p-2}0, 1^10, 1^00)\}$ in the future research. If this is true, it will support the relationship between the Laplacian coefficients and the Laplacian permanent of n-vertex bipartite unicyclic graphs with a (p,q)-bipartition.

To conclude this subsection, we determine the first, second, third smallest Laplacian permanent of graphs in $\mathscr{U}_n$, the set of all bipartite unicyclic graphs on n vertices.

THEOREM 3.11. *Among $\mathscr{U}_n$ with $n \geq 4$,*

(i) *for all $G \in \mathscr{U}_n$, we have* $\mathrm{per}L(G) \geq 24n - 60$ *with equality if and only if* $G \cong B(2, n-2)$.
(ii) *for all $G \in \mathscr{U}_n \setminus \{B(2,n-2)\}$ with $n \geq 6$, we have* $\mathrm{per}L(G) \geq 40n - 140$ *with equality if and only if* $G \cong C_4(1^10, 1^00, 1^{n-5}0, 1^00)$.
(iii) *for all $G \in \mathscr{U}_n \setminus \{B(2,n-2), C_4(1^10, 1^00, 1^{n-5}0, 1^00)\}$ with $n \geq 6$, we have* $\mathrm{per}L(G) \geq 44n - 160$ *with equality if and only if* $G \cong B(3, n-3)$.

Proof. It is routine to see that $\mathscr{U}_n = \mathscr{U}_n^{2,n-2} \cup \mathscr{U}_n^{3,n-3} \cup \cdots \cup \mathscr{U}_n^{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$. Note that for all $G \in \mathscr{U}_n^{p,q}$, by Theorem 3.8 one has $\mathrm{per}L(G) \geq \mathrm{per}L(B(p,q)) = 20(p-1)(q-1) + 4n$, with the equality if and only if $G \cong B(p,q)$. Consider the function

$$f(x) = 20(x-1)(n-x-1) + 4n$$

in x with $2 \leq x \leq \lfloor \frac{n}{2} \rfloor$. It is routine to check that $f'(x) = 20(n-2x) > 20(n-x-(n-x)) = 0$. Hence, $f(x)$ is an increasing function for $2 \leq x \leq \lfloor \frac{n}{2} \rfloor$. That is to say, $f(2) < f(3) < \cdots < f\left(\lfloor \frac{n}{2} \rfloor\right)$, which implies (i) immediately.

Based on Theorems 3.8 and 3.9, and the proof in (i) as above, in order to determine the graph in $\mathscr{U}_n$ having the second minimal Laplacian permanent, it suffices to compare the values between $\mathrm{per}L(C_4(1^10, 1^00, 1^{n-5}0, 1^00))$ and $\mathrm{per}L(B(3, n-3))$. By an elementary calculation, we have

$$\mathrm{per}L(C_4(1^10, 1^00, 1^{n-5}0, 1^00)) = 40n - 140, \quad \mathrm{per}L(B(3, n-3)) = 44n - 160. \tag{3.10}$$

It is routine to check that $\mathrm{per}L(C_4(1^10, 1^00, 1^{n-5}0, 1^00)) < \mathrm{per}L(B(3, n-3))$. Hence, (ii) holds immediately.

Similarly, in order to determine the third minimal Laplacian permanent among $\mathscr{U}_n$, it suffices to compare the values between $\mathrm{per}L(C_4(1^20, 1^00, 1^{n-6}0, 1^00))$ and

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per$L(B(3, n-3))$. Note that if $n = 6$ (resp., 7), it is straightforward to check that $C_4(1^20, 1^00, 1^{n-6}0, 1^00)$ does not exist and $B(3, n-3)$ is the graph with the third minimal Laplacian permanent among $\mathscr{U}_n$. For $n \geq 8$, by direct calculation, we have

$$\text{per}L(C_4(1^20, 1^00, 1^{n-6}0, 1^00)) = 56n - 252. \tag{3.11}$$

In view of the second equation in (3.10) and (3.11), it is routine to check that per$L(C_4(1^20, 1^00, 1^{n-6}0, 1^00)) >$ per$L(B(3, n-3)) = 44n - 160$. Hence, (iii) holds immediately. □

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