



Maximum hitting time of random walks on unicyclic graphs with given diameter

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Abstract.

We explore the extremal problems of the hitting time of unicyclic graphs on n vertices with a given diameter. Let $H_G(u, v)$ be the expected hitting time from vertex u to vertex v on a simple graph G . Let $\varphi(G) = \max_{u, v \in V(G)} H_G(u, v)$ be the hitting time of G . In this paper, we obtain the upper bound for the hitting time of unicyclic graphs with a given diameter, and the extremal graph that attained the value is determined.

1. Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The size of $V(G)$ and $E(G)$ are called the *order* and the *size* of G respectively. The *distance* between vertices x and y , denoted by $d_G(x, y)$, is the length of a shortest path joining x and y in G . The *diameter* of G , denoted by $D(G)$, is the maximum distance between any two distinct vertices in G . The *girth* of G is the length of the shortest cycle. The degree of vertex x in G , denoted by $d_G(x)$, is the number of vertices adjacent to x . If there exists only one path between vertices x and y , this path is called the *unique path* and denoted by $P = xv_1v_2 \dots v_ky$, where each v_i is a cut vertex on P . Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two simple connected graphs such that $V_1 \cap V_2 = \{x, y\}$ and $E_1 \cap E_2 = \emptyset$. The union of G_1 and G_2 , denoted by $G_1 \cup G_2$, is the graph G defined by $V(G) = V_1 \cup V_2$ and $E(G) = E_1 \cup E_2$. In this case, we say that G is decomposed into G_1 and G_2 through x and y .

Let $\mathcal{U}_{n,d}$ be the set of all n -vertex unicyclic graphs with diameter d . Let $\mathcal{U}_{n,d,g}$ be the set of all n -vertex unicyclic graphs with diameter d and girth g . Without loss of generality, the unique cycle C of length g in a unicyclic graph is denoted by $C = u_1u_2 \dots u_g$ in clockwise order. Let $G \in \mathcal{U}_{n,d,g}$. If $n = g$, then G is exactly a cycle of order n and $d = \lfloor \frac{n}{2} \rfloor$. Moreover, any unicyclic graph G in $\mathcal{U}_{n,d,g}$ can be obtained by identifying vertex u_i of C with a vertex of a tree T_i for $i = 1, \dots, g$, then G is denoted by $G = C(T_1, \dots, T_g)$. Let the order of T_i be n_i . Then $n_i \geq 1$ and $n_1 + \dots + n_g = n$. If there are some trees T_i for all $i = p, \dots, q$ and $q > p$ such

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that $n_i > 1$ and T_r for all $1 \leq r \leq g$, $i \neq p, \dots, q$ such that $n_r = 1$, then $C(T_1, \dots, T_g)$ is short for $C_g(T_p, \dots, T_q)$. For instance, if $n_p, n_q > 1$ and $n_r = 1$ for all $1 \leq r \leq g$, $i \neq p, q$, then $C(T_1, \dots, T_g)$ is short for $C_g(T_p, T_q)$. In particular, if $G = C_3(T)$, where T is obtained by identifying an end vertex of a path on d vertices and the center of the star $K_{1,n-d-2}$, then this unicyclic graph is denoted by $U_{n,d,3}^*$ i.e., $U_{n,d,3}^*$ is the graph obtained by identifying the vertex of T with degree $n - d - 1$ and a vertex of a triangle.

Random walks on graphs are a type of stochastic process where a “walker” moves from one vertex to its neighboring vertex in the graph based on a certain probability distribution. A simple random walk is such a stochastic process with a uniform probability distribution, in which each neighboring vertex has an equal probability of being chosen. The *hitting time* $H_G(x, y)$ is the expected number of steps it takes a simple random walk on a graph G from a vertex x to a vertex y . For a given graph G , the hitting time of G is denoted by

$$\varphi(G) = \max_{x,y \in V(G)} H_G(x, y).$$

Random walks on graphs have been studied extensively in the fields of mathematics, physics, computer science, statistical physics, and biology. It has applications in algorithms, network analysis, and statistical mechanics. They can be used to model the behavior of particles diffusing through a medium, to analyze the structure of networks, and to study algorithms for graph traversal and search. Hitting time, cover time, and commute time, access time are essential metrics used to analyze the behavior of simple random walks on graphs, see [1, 6–10, 12–14, 17, 20–22, 24, 25] for more details.

The study of extremal problems of random walks on graphs has garnered significant interest among academic researchers. Research on the extremal problems of hitting time, cover time, access time and cover cost has received widespread attention. Specifically, Brightwell and Winkler [5] proved that the n -vertex lollipop graph G is the extremal graph with the maximum hitting time among all n -vertex graphs. Georgakopoulos and Wagner [11] proved the n -vertex path is the extremal graph with maximum hitting time among all n -vertex trees. Li and Zhang [29, 30] solved the extremal problems of hitting time of trees with given parameters. Liao et al. [18] studied the upper and lower bounds of access time on a tree of a given diameter and presented the corresponding extremal graphs. Feng et al. [19] studied the upper and lower bounds of access time on trees that can be decomposed into independent sets, and gave the corresponding extremal graphs. Zhu and Zhang [32, 33] determined the extremal graphs among n -vertex unicyclic graphs and n -vertex bicyclic graphs and presented the sharp upper and lower bounds for the hitting time. Zhu and Yang [34] determined the extremal graphs among n -vertex tricyclic graphs and presented the sharp upper and lower bounds for the hitting time. Beveridge and Youngblood [2] characterized the extremal structures for mixing walks on trees and showed that among all trees with n -vertex, the best mixing time is minimized uniquely by the star. For even n , the best mixing time is maximized by the unique path. Surprising, for odd n , the best mixing time is maximized uniquely by a path of length $n - 1$ with a single leaf adjacent to one central vertex. Brightwell [4] investigated extremal problems of cover time on trees and proved the n -vertex path is the extremal graph with maximum cover time. Georgakopoulos and Wagner [11] determined the maximal and minimal cover cost of n -vertex trees. Li and Wang [26] characterized the unique tree with the minimum cover cost and minimum reverse cover cost among all trees with a given segment sequence. Furthermore, the unique tree with the maximal reverse cover cost among all trees with a given segment sequence is also identified. Li and Wang [27, 28] studied the extremal problems on k -ary trees and trees with a given segment sequence concerning the cover cost and reverse cover cost. Huang et al. [13] determined the maximal and minimal (reverse) cover cost of n -vertex unicyclic graphs. Zhang et al. [31] characterized the extremal graphs with the minimal (reverse) cover cost of trees with a given diameter. Lu et al. [16] obtained sharp bounds of the cover cost for n -vertex bicyclic graphs.

Inspired by the above research, we find that the extremal problems of the hitting time of random walks on graphs with given parameters are interesting and worth further investigation. In this paper, we have investigated the extremal problem of hitting times of unicyclic graphs on n vertices with given diameter d . The following theorem is the main result.

Theorem 1.1. *Let G be any unicyclic graph of order n and $D(G) = d$. Then*

$$\varphi(G) \leq 2(d-1)n - d^2 + 2d + 1.$$

Moreover, the right equality holds if and only if $G = U_{n,d,3}^*$ and $\varphi(U_{n,d,3}^*) = H_{U_{n,d,3}^*}(u, v)$, where u is the vertex on the cycle with $d_{U_{n,d,3}^*}(u) = 2$ and v is the pendant vertex with $d_{U_{n,d,3}^*}(u, v) = d$.

The rest of this paper is organized as follows. In section 2, we present the preliminary results which are used in the proof of our main results. In section 3, we demonstrate how the hitting time of unicyclic graphs on n vertices with given diameter d alters by graph transformations, as well as the proof of the main Theorem 1.1.

2. Preliminary

In this section, we present several known important results which are useful in our proof.

Theorem 2.1. [15] Let G be a connected graph with two vertices x and y . If there exists a cut vertex z such that x and y are not in the same component of $G - z$, then

$$H_G(x, y) = H_G(x, z) + H_G(z, y). \quad (1)$$

Moreover, if there exists a unique path $P = xv_1 \cdots v_{k-1}y$ in G , then

$$H_G(x, y) = H_G(x, v_1) + H_G(v_1, v_2) + \cdots + H_G(v_{k-1}, y). \quad (2)$$

Theorem 2.2. [4] Let G be a simple connected graph on n vertices with two vertices x and y . If there exists a unique path $P = v_0v_1 \cdots v_k$ with $v_0 = x$ and $v_k = y$, and m_i is the number of edges of subgraph G_i which is the component $G - \{v_{i-1}v_i, v_iv_{i+1}\}$ with containing v_i for $i = 0, \dots, k$ and $v_{-1}v_0 = \emptyset$, and $v_kv_{k+1} = \emptyset$, then

$$H_G(x, y) = k^2 + 2 \sum_{i=0}^{k-1} m_i(k-i). \quad (3)$$

Theorem 2.3. [23] Let $G = C(T_1, \dots, T_g)$ be a unicyclic graph with cycle $C = u_1 \cdots u_g$ and G_1 and G_2 be a decomposition of G through u_i and u_j for $1 \leq i \neq j \leq g$. Then

$$H_G(u_i, u_j) = \frac{1}{g} (d_{G_2}(u_i, u_j)H_{G_1}(u_i, u_j) + d_{G_1}(u_i, u_j)H_{G_2}(u_i, u_j)), \quad (4)$$

where $d_{G_i}(u_i, u_j)$ is the distance in the graph G_i between u_i and u_j for $i = 1, 2$.

Lemma 2.4. [3] Let C be a cycle of length g . Then for any $u_i, u_j \in V(C)$, we have

$$H_C(u_i, u_j) = d(u_i, u_j)(g - d(u_i, u_j)),$$

where $d(u_i, u_j)$ is the distance between u_i and u_j in C .

Lemma 2.5. Let G be a graph of order n . Let $P = v_0v_1 \cdots v_k$ be a unique path in G with $v_0 = u$ and $v_k = v$, and G_i be the component $G - \{v_{i-1}v_i, v_iv_{i+1}\}$ containing v_i for $i = 0, \dots, k$ and $v_{-1}v_0 = \emptyset$, and $v_kv_{k+1} = \emptyset$. Let G', G'', G''' (see Figure 1) be the graphs obtained from G by transformations. Then

$$(1) H_{G'}(u, v) > H_G(u, v);$$

$$(2) H_{G''}(u, v') > H_G(u, v);$$

$$(3) H_{G'''}(u, v) > H_G(u, v).$$

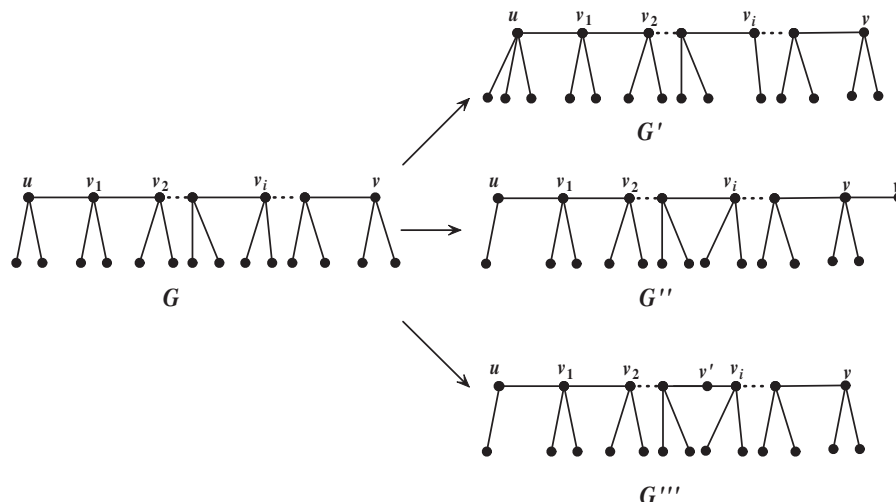


Figure 1: Transformation I

Proof. (1). By Figure 1, we see that G' is obtained by deleting a pendant edge in G_i and adding it to vertex u . Denote the size of G_i by m_i and we assume that $m_i \geq 1$ without loss of generality. By Theorem 2.2, we have

$$\begin{aligned} H_G(u, v) &= k^2 + 2m_0k + 2m_1(k-1) + \cdots + 2m_i(k-i) + \cdots + 2m_{k-1}, \\ H_{G'}(u, v) &= k^2 + 2(m_0+1)k + 2m_1(k-1) + \cdots + 2(m_i-1)(k-i) + \cdots + 2m_{k-1}. \end{aligned}$$

Since $H_{G'}(u, v) - H_G(u, v) = 2i > 0$, we have $H_{G'}(u, v) > H_G(u, v)$.

(2). By Figure 1, we see that G'' is obtained from G by deleting a pendant edge in G_0 and adding it to vertex v . Denote the newly added edge by vv' . Without loss of generality, we assume that $m_0 \geq 1$. By Theorem 2.2, we have

$$\begin{aligned} H_G(u, v) &= k^2 + 2m_0k + \cdots + 2m_i(k-i) + \cdots + 2m_{k-1}, \\ H_{G''}(u, v') &= (k+1)^2 + 2(m_0-1)(k+1) + \cdots + 2m_i(k+1-i) + \cdots + 2m_{k-1} \cdot 2 + 2m_k. \end{aligned}$$

Since $H_{G''}(u, v') - H_G(u, v) = 2 \sum_{i=0}^k m_i - 1 > 0$, we have $H_{G''}(u, v') > H_G(u, v)$.

(3). By Figure 1, we see that G''' is obtained from G by deleting a pendant edge in G_0 and inserting a vertex in P . Without loss of generality, we assume that $m_0 \geq 1$ and the inserted vertex is v' and the new path is $P = v_0v_1 \dots v'v_i \dots v_k$. By Theorem 2.2, we have

$$\begin{aligned} H_G(u, v) &= k^2 + 2m_0k + \cdots + 2m_{i-1}(k-i+1) + 2m_i(k-i) + \cdots + 2m_{k-1}, \\ H_{G'''}(u, v) &= (k+1)^2 + 2(m_0-1)(k+1) + \cdots + 2m_{i-1}(k-i+2) + 2m_i(k-i) + \cdots + 2m_{k-1}. \end{aligned}$$

Since $H_{G'''}(u, v) - H_G(u, v) = 2 \sum_{t=0}^{i-1} m_t - 1 > 0$, we have $H_{G'''}(u, v) > H_G(u, v)$. $\square$

3. The Proof of Theorem 1.1

To prove Theorem 1.1, we first present several lemmas about how the hitting time changes after graph transformation.

As observed before, if $G \in \mathcal{U}_{n,d,g}$ with $n = g$, then G is the unique cycle of order n , and there is no graph transformation. Therefore, we suppose that $n > g$ is the left. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$. If G' is obtained from G by deleting edges in T_i and adding edges to T_j , then $G' = C(T_1, \dots, T'_i, \dots, T'_j, \dots, T_g)$ and we simply denote $G' = C(T_{i \rightarrow j})$ for convenience.

Lemma 3.1. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ with cycle $C = u_1 \dots u_g$. Let u, v be two pendant vertices in G with $d_G(u, v) = d$ and $u \in V(T_i), v \in V(T_j)$ for $|V(T_i)| \geq 2$. Let vertex w be the unique vertex adjacent to u . Let $|V(T_p)| \geq 2$ for $p \neq i, j$. Let G' be the unicyclic graph obtained from G by deleting a pendant edge e in T_p and adding it to vertex w in T_i (see Figure 2). Then

$$H_{G'}(u, v) > H_G(u, v). \quad (5)$$

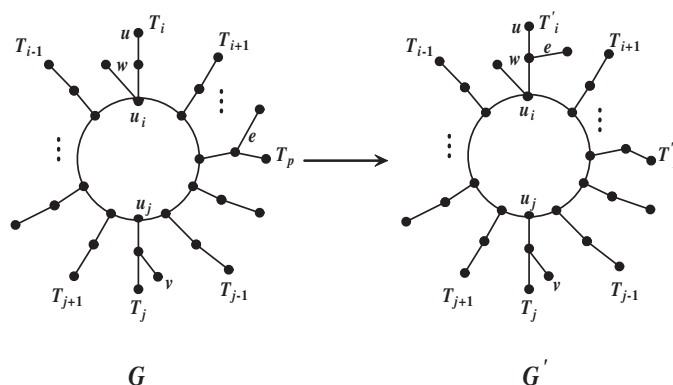


Figure 2: Transformation II

Proof. By the transformation, we can see that $D(G') = d$ and $G' = C(T_{p \rightarrow i})$. T_i and T_j can divide the cycle into two parts. There is no essential difference in the calculation in either part. Therefore, without loss of generality, we assume that $2 < i < p < j < g$. Let G_1 and G_2 be two decomposed connected subgraphs of G through two vertices u_i and u_j , where G_1 contains $T_i, T_{i+1}, \dots, T_p, \dots, T_j$. Let m_r be the size of T_r for $1 \leq r \leq g$. Moreover, let $d_{G_1}(u_i, u_j) = g_1$ and $d_{G_2}(u_i, u_j) = g_2$. By Equation (2) in Theorem 2.1, we have

$$\begin{aligned} H_G(u, v) &= H_G(u, u_i) + H_G(u_i, u_j) + H_G(u_j, v), \\ H_{G'}(u, v) &= H_{G'}(u, u_i) + H_{G'}(u_i, u_j) + H_{G'}(u_j, v). \end{aligned}$$

After the transformation, $|E(T'_i)| = |E(T_i)| + 1$. Since $d_G(u, u_i) = d_{G'}(u, u_i)$, by Equation (3) in Theorem 2.2, we have $H_G(u, u_i) < H_{G'}(u, u_i)$.

By Equation (4) in Theorem 2.3, we have

$$\begin{aligned} H_G(u_i, u_j) &= \frac{1}{g} (d_{G_2}(u_i, u_j)H_{G_1}(u_i, u_j) + d_{G_1}(u_i, u_j)H_{G_2}(u_i, u_j)) \\ &= \frac{1}{g} (g_2H_{G_1}(u_i, u_j) + g_1H_{G_2}(u_i, u_j)). \end{aligned} \quad (6)$$

Furthermore, by Equation (3) in Theorem 2.2, we have

$$\begin{aligned} H_{G_1}(u_i, u_j) &= g_1^2 + 2(m_i \cdot g_1 + m_{i+1}(g_1 - 1) + \dots + m_p(g_1 - p + i) + \dots + m_{j-1}), \\ H_{G_2}(u_i, u_j) &= g_2^2 + 2(m_{i-1}(g_2 - 1) + m_{i-2}(g_2 - 2) + \dots + m_{j+1}). \end{aligned}$$

Let G'_1 and G'_2 be a decomposition of G' through u_i and u_j such that $G'_2 = G_2$. By Equation (4) in Theorem 2.3,

$$\begin{aligned} H_{G'}(u_i, u_j) &= \frac{1}{g} (d_{G'_2}(u_i, u_j)H_{G'_1}(u_i, u_j) + d_{G'_1}(u_i, u_j)H_{G'_2}(u_i, u_j)) \\ &= \frac{1}{g} (g_2H_{G'_1}(u_i, u_j) + g_1H_{G_2}(u_i, u_j)). \end{aligned} \quad (7)$$

Moreover, by Equation (3) in Theorem 2.2, we have

$$H_{G'_1}(u_i, u_j) = g_1^2 + 2((m_i + 1)g_1 + m_{i+1}(g_1 - 1) + m_{i+2}(g_1 - 2) + \cdots + (m_p - 1)(g_1 - p + i) + \cdots + m_{j-1}).$$

Hence, by Equations (6) and (7), we have

$$\begin{aligned} H_{G'}(u_i, u_j) - H_G(u_i, u_j) &= \frac{g_2}{g} (H_{G'_1}(u_i, u_j) - H_{G_1}(u_i, u_j)) \\ &= \frac{2g_2(p - i)}{g} > 0. \end{aligned}$$

Since $T_j = T'_j$, by (3) in Theorem 2.2, we have $H_G(u_j, v) = H_{G'}(u_j, v)$. So the assertion holds. $\square$

Remark 3.2. In Lemma 3.1, if $d_G(u, v) < d$ and the graph transformation remains the diameter the same, then the conclusion of the lemma also holds.

Lemma 3.3. [32] Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$. If there exist two vertices $u, v \in V(G)$ such that $\varphi(G) = H_G(u, v)$, then u and v are either pendant vertices in $V(G)$ or vertices with degree 2 in $V(G)$, respectively.

Next, we will present how the hitting time changes between two vertices by graph transformation. Let $G \in \mathcal{U}_{n,d,g}$ and $\varphi(G) = H_G(u, v)$. In Subsection 3.1 (resp. Subsection 3.2), while $d_G(u, v) = d$ (resp. $d_G(u, v) < d$), we discuss that how the hitting time $H_G(u, v)$ changes by graph transformation.

3.1. While $d_G(u, v) = d$ and $H_G(u, v) = \varphi(G)$, how the hitting time changes by graph transformation

Lemma 3.4. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ with $n > d + g$. There exist two vertices $u \in V(T_i)$ and $v \in V(T_j)$ with $d_G(u, v) = d$ such that $H_G(u, v) = \varphi(G)$. Let $|V(T_i)| \geq 2$ and $|V(T_j)| \geq 2$ and w be the adjacent vertex of u . Let $G^1 = C_g(T_i^1, T_j^1)$ and $G^2 = C_g(T_i^2, T_j^2)$ be two graphs obtained from G by graph transformation (see Figure 3). Then

$$H_{G^2}(u, v) > H_{G^1}(u, v) > H_G(u, v). \quad (8)$$

Moreover,

$$\varphi(G^2) > \varphi(G). \quad (9)$$

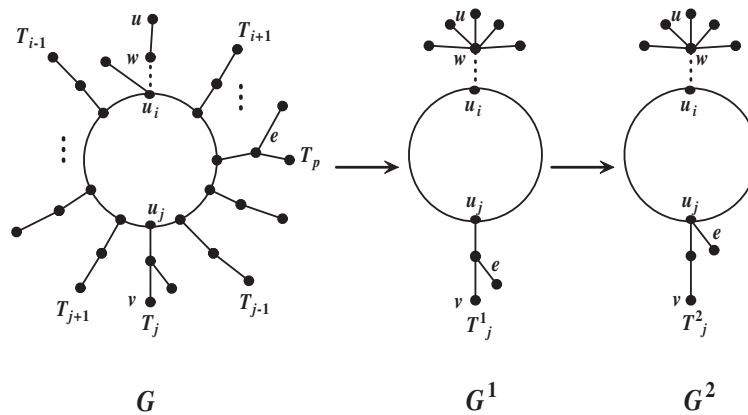


Figure 3: Transformation III

Proof. According to Figure 3, we can see that T_i^1 is the tree obtained from G by deleting all edges in T_r for all $1 \leq r \neq i, j \leq g$, and deleting all edges in T_i which do not belong to the unique path $P_1 = uw \dots u_i \in T_i$, then adding $n - g - |V(T_j)| + 1 - d_G(u, u_i)$ pendant edges to vertex w , T_j^2 is the tree obtained from T_j^1 by deleting all edges in T_j^1 which do not belong to the unique path $P_2 = u_j \dots v \in T_j^1$ and adding $|V(T_j)| - 1 - d_G(u_j, v)$ pendant edges to vertex u_j . In particular, $T_j^1 = T_j$ and $T_i^2 = T_i^1$. Without loss of generality, we assume that $|V(T_i)| \geq 2$ and $|V(T_j)| \geq 2$. By Theorem 2.1, we have

$$\begin{aligned} H_G(u, v) &= H_G(u, u_i) + H_G(u_i, u_j) + H_G(u_j, v), \\ H_{G^1}(u, v) &= H_{G^1}(u, u_i) + H_{G^1}(u_i, u_j) + H_{G^1}(u_j, v), \\ H_{G^2}(u, v) &= H_{G^2}(u, u_i) + H_{G^2}(u_i, u_j) + H_{G^2}(u_j, v). \end{aligned}$$

By repeating usage of Lemma 3.1, we have $H_{G^1}(u, v) > H_G(u, v)$. On the one hand, by repeating usage of Lemma 2.5, we have $H_{G^2}(u_j, v) > H_{G^1}(u_j, v)$. On the other hand, $H_{G^1}(u, u_i) = H_{G^2}(u, u_i)$ and $H_{G^1}(u_i, u_j) = H_{G^2}(u_i, u_j)$, then $H_{G^2}(u, v) > H_{G^1}(u, v)$. Therefore, $\varphi(G^2) \geq H_{G^2}(u, v) > H_{G^1}(u, v) > H_G(u, v) = \varphi(G)$. $\square$

Building upon Lemma 3.4, we proceed to further graph transformation on the graph G^2 , yielding the following lemma.

Lemma 3.5. Let $G^2 = C_g(T_i^2, T_j^2) \in \mathcal{U}_{n,d,g}$ be the same graph as in Lemma 3.4. Let $u \in V(T_i^2)$ and $v \in V(T_j^2)$ be two pendant vertices of G^2 with $d_{G^2}(u, v) = d$. Let $G^3 = C_g(T_i^3, T_j^3)$ be the graph obtained from G^2 by transformation (see Figure 4). Then

$$H_{G^3}(u, v) \geq H_{G^2}(u, v), \quad \varphi(G^3) \geq \varphi(G).$$

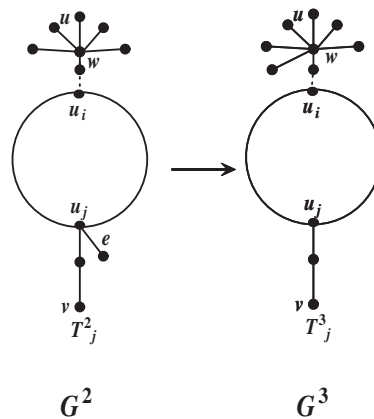


Figure 4: Transformation IV

Proof. According to Figure 4, we can see that G^3 is obtained by deleting all the pendant edges incident with u_j which are not in the path $P_{u_j v}$ from T_j^2 and adding $|V(T_j^2)| - 1 - d_{G^2}(u_j, v)$ pendant edges to vertex w , where w is the unique adjacent vertex of vertex u . By Theorem 2.1, we have

$$\begin{aligned} H_{G^2}(u, v) &= H_{G^2}(u, u_i) + H_{G^2}(u_i, u_j) + H_{G^2}(u_j, v), \\ H_{G^3}(u, v) &= H_{G^3}(u, u_i) + H_{G^3}(u_i, u_j) + H_{G^3}(u_j, v). \end{aligned}$$

Let m'_0 be the number of pendant edges incident with vertex w in T_i^2 . Let $d_{G^2}(u, u_i) = d_{G^3}(u, u_i) = d_1$, $d_{G^2}(u_j, v) = d_{G^3}(u_j, v) = d_2$, and $|V(T_j^2)| - 1 - d_2 = N$. Let G_1 and G_2 be two decomposed connected subgraphs

of G^2 through two vertices u_i and u_j such that G_1 contains T_i^2, T_j^2 . Moreover, let $d_{G_1}(u_i, u_j) = g_1, d_{G_2}(u_i, u_j) = g_2$. By Theorems 2.2 and 2.3, we have

$$\begin{aligned} H_{G^2}(u, u_i) &= d_1^2 + 2(m'_0 - 1)(d_1 - 1), \\ H_{G^2}(u_i, u_j) &= \frac{1}{g} \left(g_2 (g_1^2 + 2(d_1 + m'_0 - 1)g_1) + g_1 g_2^2 \right), \\ H_{G^2}(u_j, v) &= d_2^2 + 2(n - d_2)d_2. \end{aligned}$$

Similar to the computation of $H_{G^2}(u, v)$, we can get

$$\begin{aligned} H_{G^3}(u, u_i) &= d_1^2 + 2(m'_0 - 1 + N)(d_1 - 1), \\ H_{G^3}(u_i, u_j) &= \frac{1}{g} \left(g_2 (g_1^2 + 2(d_1 + m'_0 - 1 + N)g_1) + g_1 g_2^2 \right), \\ H_{G^3}(u_j, v) &= d_2^2 + 2(n - d_2)d_2. \end{aligned}$$

Hence, $H_{G^3}(u, v) - H_{G^2}(u, v) = 2N(d_1 - 1) + \frac{2g_1 g_2 N}{g} \geq 0$. Thus, $\varphi(G^3) \geq H_{G^3}(u, v) \geq H_{G^2}(u, v)$. Therefore, by Lemma 3.4, $\varphi(G^3) \geq \varphi(G)$. So the assertion holds. $\square$

Building upon Lemma 3.5, we compare $H_{G^3}(u, v)$ with $\varphi(U_{n,d,3}^*)$, yielding the following lemma.

Lemma 3.6. Let $G^3 = C_g(T_i^3, T_j^3) \in \mathcal{U}_{n,d,g}$ be the same graph as in Lemma 3.5. If $u \in V(T_i^3)$ and $v \in V(T_j^3)$ are two pendant vertices of G^3 with $d_{G^3}(u, v) = d$, then

$$\varphi(U_{n,d,3}^*) > H_{G^3}(u, v).$$

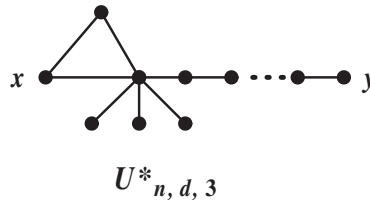


Figure 5: $U_{n,d,3}^*$

Proof. Note that $U_{n,d,3}^*$ is the graph obtained by identifying an end vertex of path P_{d-1} and a vertex in K_3 and the center of star $K_{1,n-d-2}$ (see Figure 5). By Theorems 2.1, 2.2 and 2.3; Lemmas 2.4 and 3.3; and direct computation, we obtain that $\varphi(U_{n,d,3}^*) = H_{U_{n,d,3}^*}(x, y) = 2(d-1)n - (d-1)^2 + 2$, x is a vertex in triangle with degree 2 and y is a pendant vertex with $d_{U_{n,d,3}^*}(x, y) = d$.

Let $d_{G^3}(u, u_i) = d_1, d_{G^3}(u_j, v) = d_2, d_{G^3}(u_i, u_j) = g_1$ and $g - g_1 = g_2$. Similar to the computation of $H_{G^3}(u, v)$ in Lemma 3.5, by $d_1 + d_2 + g_1 = d$, we have

$$\begin{aligned} H_{G^3}(u, v) &= d_1^2 + 2(d_1 - 1)(n - d_1 - d_2 - g) + g_1 g_2 + \frac{2g_1 g_2 (n - d_2 - g)}{g} + d_2^2 + 2(n - d_2)d_2 \\ &= 2 \left(d_1 + d_2 - 1 + \frac{g_1 g_2}{g} \right) n - d_1^2 - d_2^2 - 2d_1 d_2 + 2d_1 + 2d_2 - 2g d_1 + 2g - \frac{2g_1 g_2 d_2}{g} - g_1 g_2. \end{aligned} \quad (10)$$

Since $n \geq d_1 + d_2 + g$ and $d_1 \geq 1$, we have

$$\varphi(U_{n,d,3}^*) - H_{G^3}(u, v) = 2 \left(d - d_1 - d_2 - \frac{g_1 g_2}{g} \right) n - (d-1)^2 + 2 + d_1^2 + d_2^2$$

$$\begin{aligned}
& +2d_1d_2 - 2d_1 - 2d_2 + 2gd_1 - 2g + \frac{2g_1g_2d_2}{g} + g_1g_2 \\
= & 2\left(d - d_1 - d_2 - \frac{g_1g_2}{g}\right)n - (d + d_1 + d_2 - 2)(d - d_1 - d_2) \\
& + 1 + 2gd_1 - 2g + \frac{2g_1g_2d_2}{g} + g_1g_2 \\
= & \frac{2g_1^2}{g}n - g_1^2 - 2d_2g_1 - 2g_2 + 2g_2d_1 + \frac{2g_1g_2d_2}{g} + g_1g_2 + 1 \\
\geq & \frac{2g_1^2(d_1 + d_2 + g)}{g} - g_1^2 - 2d_2g_1 - 2g_2 + 2g_2d_1 + \frac{2g_1g_2d_2}{g} + g_1g_2 + 1 \\
= & \frac{2g_1^2d_1}{g} + 2g_2(d_1 - 1) + g_1^2 + g_1g_2 + 1 \\
> & 0.
\end{aligned} \tag{11}$$

So the assertion holds. $\square$

In the above lemmas, with the condition $\varphi(G) = H_G(u, v)$, we have discussed how the hitting time $H_G(u, v)$ changes by graph transformation while $d_G(u, v) = d$ and $u \in V(T_i)$ for $|V(T_i)| \geq 2$. In particular, if $d_G(v) = 2$, by deleting v , the graph is divided into two parts. The part without the cycle does not affect $H_G(u, v)$, so the above calculation process still holds. However, when $d_G(u) = 2$, the graph transformation in the above lemmas is invalid. Therefore, when $d_G(u) = 2$ and $d_G(u, v) = d$, it needs to be discussed separately. The following lemmas and corollary will discuss how the hitting time $H_G(u, v)$ changes by graph transformation while $d_G(u, v) = d$ and $u \in V(T_i)$ for $|V(T_i)| = 1$.

Lemma 3.7. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ where $T_i = u_i = u$. If there exists vertex v with $v \in V(T_j)$ such that $d_G(u, v) = d$ and $\varphi(G) = H_G(u, v)$, then we have the following results.

- (1) If g is even and $G' = C(T_{p \rightarrow i+1}) \in \mathcal{U}_{n,d,g}$ is obtained from G by deleting the pendant edge e in T_p and adding it to the vertex u_{i+1} (see Figure 6), then

$$H_{G'}(u, v) > H_G(u, v) \quad \text{and} \quad \varphi(G') \geq \varphi(G). \tag{12}$$

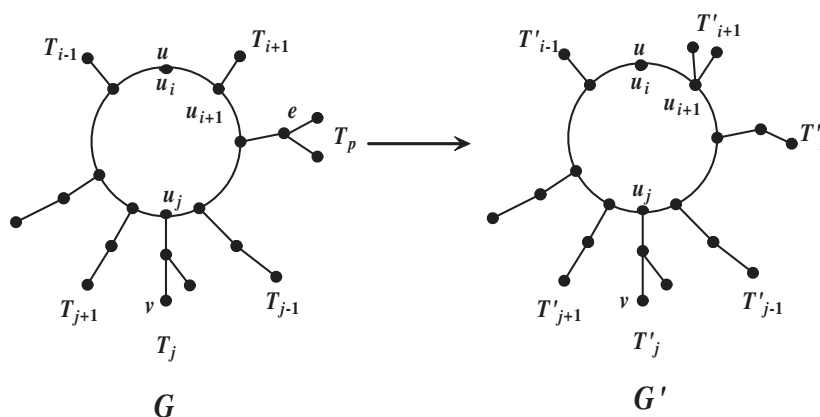


Figure 6: Transformation V

- (2) If g is odd and $G'' = C(T_{p \rightarrow i+2}) \in \mathcal{U}_{n,d,g}$ is obtained from G by deleting the pendant edge e in T_p and adding it to the vertex u_{i+2} (see Figure 7), then

$$H_{G''}(u, v) > H_G(u, v) \quad \text{and} \quad \varphi(G'') \geq \varphi(G). \quad (13)$$

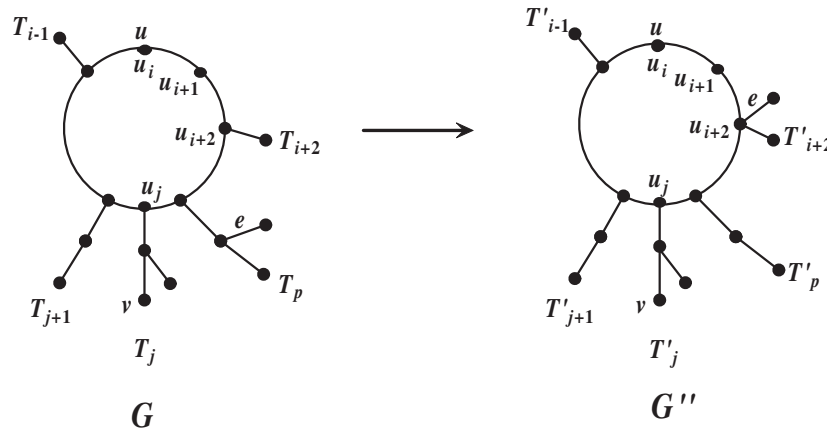


Figure 7: Transformation VI

Proof. (1) Since g is even and $d_G(u, v) = d$, we have $d_G(u, u_j) = \frac{g}{2}$, T_{i+1} and T_{i-1} are stars or single vertices. Without loss of generality, we assume that $2 < i < p < j < g$. Let G_1 and G_2 be two decomposed connected subgraphs of G through two vertices u_i and u_j where G_1 contains $T_i, T_{i+1}, \dots, T_p, \dots, T_j$. Let m_r be the size of T_r for all r and $1 \leq r \leq g$. Moreover, let $d_{G_1}(u_i, u_j) = g_1$, $d_{G_2}(u_i, u_j) = g_2$. Then $g_1 = g_2 = \frac{g}{2}$. By (2) in Theorem 2.1, we have

$$\begin{aligned} H_G(u, v) &= H_G(u, u_j) + H_G(u_j, v), \\ H_{G'}(u, v) &= H_{G'}(u, u_j) + H_{G'}(u_j, v). \end{aligned}$$

By Equation (4) in Theorem 2.3, we have

$$\begin{aligned} H_G(u, u_j) &= \frac{1}{g} (d_{G_2}(u, u_j)H_{G_1}(u, u_j) + d_{G_1}(u, u_j)H_{G_2}(u, u_j)) \\ &= \frac{1}{2} (H_{G_1}(u, u_j) + H_{G_2}(u, u_j)). \end{aligned} \quad (14)$$

Furthermore, by Equation (3) in Theorem 2.2, we have

$$\begin{aligned} H_{G_1}(u, u_j) &= g_1^2 + 2(m_{i+1}(g_1 - 1) + \dots + m_p(g_1 - p + i) + \dots + m_{j-1}), \\ H_{G_2}(u, u_j) &= g_2^2 + 2(m_{i-1}(g_2 - 1) + m_{i-2}(g_2 - 2) + \dots + m_{j+1}). \end{aligned}$$

Let G'_1 and G'_2 be a decomposition of G' through u_i and u_j such that $G'_2 = G_2$. By (3) in Theorem 2.2,

$$\begin{aligned} H_{G'}(u, u_j) &= \frac{1}{g} (d_{G'_2}(u, u_j)H_{G'_1}(u, u_j) + d_{G'_1}(u, u_j)H_{G'_2}(u, u_j)) \\ &= \frac{1}{2} (H_{G'_1}(u, u_j) + H_{G_2}(u, u_j)). \end{aligned} \quad (15)$$

Moreover, by (4) in Theorem 2.3, we have

$$H_{G'_1}(u, u_j) = g_1^2 + 2((m_{i+1} + 1)(g_1 - 1) + m_{i+2}(g_1 - 2))$$

$$+ \cdots + (m_p - 1)(g_1 - p + i) + \cdots + m_{j-1}).$$

Hence, by Equations (14) and (15), we have

$$\begin{aligned} H_{G'}(u, u_j) - H_G(u, u_j) &= \frac{1}{2} (H_{G'_i}(u, u_j) - H_{G_1}(u, u_j)) \\ &= p - i - 1 > 0. \end{aligned}$$

Since $T_j = T'_j$, by (3) in Theorem 2.2, we have $H_G(u_j, v) = H_{G'}(u_j, v)$. So the assertion holds.

(2) Since $d_G(u, v) = d$, we have $d_G(u, u_j) = \frac{g-1}{2}$, T_{i+1} is a single vertex, T_{i-1} and T_{i+2} are stars or single vertices. Similar to the proof in (1), by computation, we can get the result. $\square$

Lemma 3.8. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ where $T_i = u_i = u$. If there exists vertex v with $v \in V(T_j)$ such that $d_G(u, v) = d$ and $\varphi(G) = H_G(u, v)$, then we have the following results.

(1) If g is even and $G'' = C(T''_{i-1}, T''_{i+1}, T''_j)$ with $T''_{i+1} = K_{1,s}$, $T''_{i-1} = K_{1,t}$, $T''_j = P_{u_j v}$ (see Figure 8), then

$$\varphi(U_{n,d,3}^*) > H_{G''}(u, v) > \varphi(G). \quad (16)$$

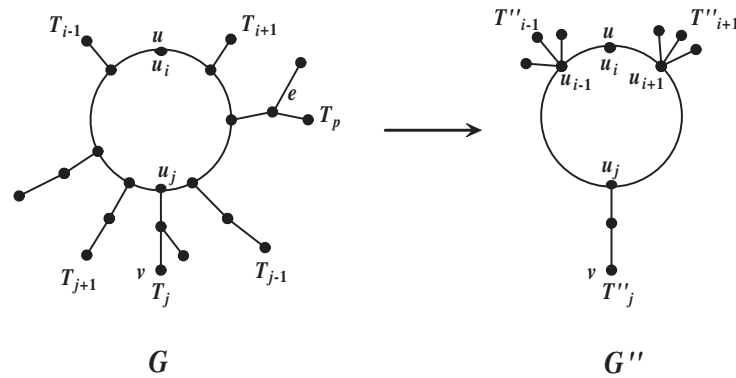


Figure 8: Transformation VII

(2) If g is odd and $G'' = C(T''_{i-1}, T''_{i+2}, T''_j)$ with $T''_{i-1} = K_{1,s}$, $T''_{i+2} = K_{1,t}$, $T''_j = P_{u_j v}$ (see Figure 9), then

$$\varphi(U_{n,d,3}^*) > H_{G''}(u, v) > \varphi(G). \quad (17)$$

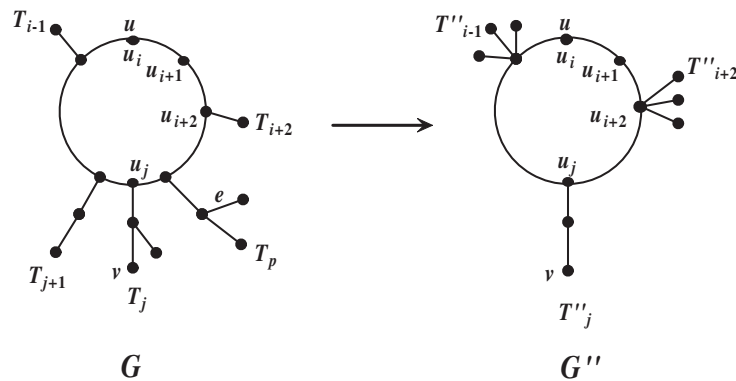


Figure 9: Transformation VIII

Proof. (1) Without loss of generality, we assume that $2 < i < p < j < g$. The graph G'' can be obtained from G by graph transformation.

In the first step, we can delete all the edges of $T_{i+2}, T_{i+3}, \dots, T_{j-1}$ in G and add these edges to vertex u_{i+1} , then we get a new graph G^{1*} . We denote $G^{1*} = C(T_1^{1*}, \dots, T_g^{1*})$. By repeating usage of (1) in Lemma 3.7, we have $H_{G^{1*}}(u, v) > H_G(u, v)$.

The second step, we can delete all the edges of $T_{j+1}^{1*}, T_{j+2}^{1*}, \dots, T_{i-2}^{1*}$ in G^{1*} and add these edges to vertex u_{i-1} , then we get a new graph G^{2*} . We denote $G^{2*} = C(T_1^{2*}, \dots, T_g^{2*})$. By repeating usage of (1) in Lemma 3.7, we have $H_{G^{2*}}(u, v) > H_{G^{1*}}(u, v)$.

In the third step, we can delete all the edges of T_j^{2*} in G^{2*} which do not belong to the u_jv -path and add these edges to u_j , then we get a new graph G^{3*} . We denote $G^{3*} = C(T_1^{3*}, \dots, T_g^{3*})$. By repeating usage of Lemma 2.5, we have $H_{G^{3*}}(u, v) > H_{G^{2*}}(u, v)$.

The fourth step, we delete the pendent edges of T_j^{3*} in G^{3*} which do not belong to the u_jv -path and add these edges to u_{i-1} or u_{i+1} . After the above four steps, we get the graph G'' . We denote $G'' = C(T_{i-1}'', T_{i+1}'', T_j'')$, where $T_{i+1}'' = K_{1,s}$, $T_{i-1}'' = K_{1,t}$, $T_j'' = P_{u_jv}$. By Theorem 2.1, we have

$$H_{G^{3*}}(u, v) = H_{G^{3*}}(u, u_j) + H_{G^{3*}}(u_j, v)$$

and

$$H_{G''}(u, v) = H_{G''}(u, u_j) + H_{G''}(u_j, v).$$

By Theorems 2.2, 2.3 and similar to the computation in Lemma 3.5, we have $H_{G''}(u, u_j) > H_{G^{3*}}(u, u_j)$ and $H_{G^{3*}}(u_j, v) = H_{G''}(u_j, v)$. Hence, $H_{G''}(u, v) > H_{G^{3*}}(u, v)$. Therefore, $H_{G''}(u, v) > H_G(u, v)$.

Let $d_{G''}(u_j, v) = d_2$. By Theorems 2.1, 2.2 and 2.3 and $d_2 = d - \lfloor \frac{g}{2} \rfloor$, we have

$$H_{G''}(u, v) = H_{G''}(u, u_j) + H_{G''}(u_j, v).$$

If g is even, then

$$\begin{aligned} H_{G''}(u, v) &= \frac{g^2}{4} + (n - g - d_2) \left(\frac{g}{2} - 1 \right) + 2d_2n - d_2^2 \\ &= \left(2d - 1 - \frac{g}{2} \right) n + \frac{g + dg}{2} - \frac{g^2}{4} + d - d^2. \end{aligned}$$

Since $\varphi(U_{n,d,3}^*) = 2(d-1)n - (d-1)^2 + 2$ and $n \geq d + \lfloor \frac{g}{2} \rfloor$, we have

$$\begin{aligned} \varphi(U_{n,d,3}^*) - H_{G''}(u, v) &= \left(\frac{g}{2} - 1 \right) n + d + 1 + \frac{g^2}{4} - \frac{g}{2} - \frac{dg}{2} \\ &\geq \left(\frac{g}{2} - 1 \right) \left(d + \frac{g}{2} \right) + d + 1 + \frac{g^2}{4} - \frac{g}{2} - \frac{dg}{2} \\ &= \frac{g^2}{2} - g + 1 \\ &> 0. \end{aligned}$$

Therefore, we have $\varphi(U_{n,d,3}^*) \geq H_{G''}(u, v) > \varphi(G)$.

(2) Similar to the frontier proof in (1), we can prove that $H_{G''}(u, v) > \varphi(G)$. If g is odd, then

$$H_{G''}(u, v) \leq \frac{g^2 - 1}{4} + \left(n - d - \frac{g + 1}{2} \right) \frac{g^2 - 2g - 3}{2g} + 2 \left(d - \frac{g - 1}{2} \right) n - \left(d - \frac{g - 1}{2} \right)^2$$

and

$$\varphi(U_{n,d,3}^*) - H_{G''}(u, v) \geq \frac{(g^2 - 4g + 3)n}{2g} - (d - 1)^2 + 2 - \frac{g^2 - 1}{4}$$

$$\begin{aligned}
& + \frac{g^2 - 2g - 3}{2g} \left(d + \frac{g+1}{2} \right) + \left(d - \frac{g-1}{2} \right)^2 \\
\geq & \frac{g^2 - 4g + 3}{2g} \left(d + \frac{g-1}{2} \right) - (d-1)^2 + 2 - \frac{g^2 - 1}{4} \\
& + \frac{g^2 - 2g - 3}{2g} \left(d + \frac{g+1}{2} \right) + \left(d - \frac{g-1}{2} \right)^2 \\
\geq & (g-3) \left(d + \frac{g-1}{2} \right) - (d-1)^2 + 2 - \frac{g^2 - 1}{4} + \left(d - \frac{g-1}{2} \right)^2 \\
= & \frac{(g-2)(g-3)}{2} \\
\geq & 0.
\end{aligned}$$

Therefore, we have $\varphi(U_{n,d,3}^*) \geq H_{G''}(u, v) > \varphi(G)$. $\square$

3.2. While $d_G(u, v) < d$ and $H_G(u, v) = \varphi(G)$, how the hitting time changes by graph transformation

Let $G^3 = C(T_1^3, \dots, T_g^3) \in \mathcal{U}_{n,d,g}$, where T_i^3 is the tree obtained from identifying an end vertex of a path and the center of a star and T_j^3 is a path. Let $u \in V(T_i^3)$ and $v \in V(T_j^3)$. Let u and v be two pendant vertices or vertices on the cycle with degree 2. We have,

1. if $d_{G^3}(u, v) < d$, $d_{G^3}(u_j, v) + \left\lfloor \frac{g}{2} \right\rfloor < d$ and $d_{G^3}(u_i, u) + \left\lfloor \frac{g}{2} \right\rfloor = d$, then we denote G^3 by $\widetilde{G}^3$ and T_s by $\widetilde{T}_s^3$ for $s = 1, \dots, g$.
2. if $d_{G^3}(u, v) < d$, $d_{G^3}(u_j, v) + \left\lfloor \frac{g}{2} \right\rfloor = d$ and $d_{G^3}(u_i, u) + \left\lfloor \frac{g}{2} \right\rfloor < d$, then we denote G^3 by $\overline{G}^3$ and T_s by $\overline{T}_s^3$ for $s = 1, \dots, g$.
3. if $d_{G^3}(u, v) < d$, $d_{G^3}(u_j, v) + \left\lfloor \frac{g}{2} \right\rfloor = d$ and $d_{G^3}(u_i, u) + \left\lfloor \frac{g}{2} \right\rfloor = d$, then we denote G^3 by $\widehat{G}^3$ and T_s by $\widehat{T}_s^3$ for $s = 1, \dots, g$.
4. if $d_{G^3}(u, v) < d$, $d_{G^3}(u, u_i) + \left\lfloor \frac{g}{2} \right\rfloor = d$ or $d_{G^3}(u_j, v) + \left\lfloor \frac{g}{2} \right\rfloor = d$ and T_i^3 and T_j^3 are paths, then we denote G^3 by G^{3*} and T_s by T_s^{3*} for $s = 1, \dots, g$.

Lemma 3.9. Let $G^3 = C(T_1^3, \dots, T_g^3) \in \mathcal{U}_{n,d,g}$ be the graph obtained from $\widetilde{G}^3$ by deleting one pendant edge from the vertex w in $\widetilde{T}_i^3$ and adding the edge to the pendant vertex v in $\widetilde{T}_j^3$. Let $T_j^3 = P_{u_j v'}$ (See Figure 10). Then

$$H_{G^3}(u, v') > H_{\widetilde{G}^3}(u, v).$$

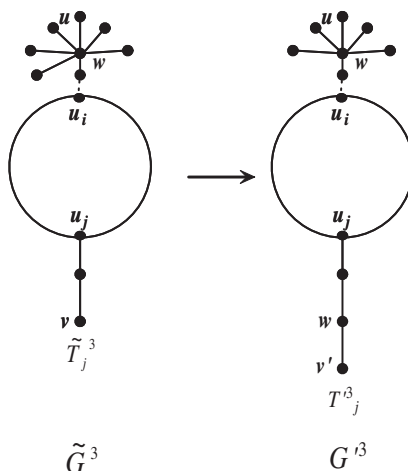


Figure 10: Transformation IX

Proof. By Theorem 2.1, we have

$$H_{\tilde{G}^3}(u, v) = H_{\tilde{G}^3}(u, u_i) + H_{\tilde{G}^3}(u_i, u_j) + H_{\tilde{G}^3}(u_j, v),$$

and

$$H_{G'^3}(u, v') = H_{G'^3}(u, u_i) + H_{G'^3}(u_i, u_j) + H_{G'^3}(u_j, v').$$

Let m'_0 be the number of pendant edges incident with vertex w in $\tilde{T}_i^3$. Let $d_{\tilde{G}^3}(u, u_i) = d_{G'^3}(u, u_i) = d_1$, $d_{\tilde{G}^3}(u_j, v) = d_2$. Let G_1 and G_2 be two decomposed connected subgraphs of $\tilde{G}^3$ through two vertices u_i and u_j such that G_1 contains $\tilde{T}_i^3, \tilde{T}_j^3$. Moreover, let $d_{G_1}(u_i, u_j) = g_1$, $d_{G_2}(u_i, u_j) = g_2$. By Theorems 2.2 and 2.3, we have

$$\begin{aligned} H_{\tilde{G}^3}(u, u_i) &= d_1^2 + 2(m'_0 - 1)(d_1 - 1), \\ H_{\tilde{G}^3}(u_i, u_j) &= \frac{1}{g} (g_2(g_1^2 + 2(d_1 + m'_0 - 1)g_1) + g_1g_2^2), \\ H_{\tilde{G}^3}(u_j, v) &= d_2^2 + 2(n - d_2)d_2. \end{aligned}$$

Similar to the computation of $H_{\tilde{G}^3}(u, v)$, we can get

$$\begin{aligned} H_{G'^3}(u, u_i) &= d_1^2 + 2(m'_0 - 2)(d_1 - 1), \\ H_{G'^3}(u_i, u_j) &= \frac{1}{g} (g_2(g_1^2 + 2(d_1 + m'_0 - 2)g_1) + g_1g_2^2), \\ H_{G'^3}(u_j, v) &= (d_2 + 1)^2 + 2(n - d_2 - 1)(d_2 + 1). \end{aligned}$$

Since $n \geq g + d_1 + d_2$, we have $H_{G'^3}(u, v') - H_{\tilde{G}^3}(u, v) = \frac{2(gn - gd_1 - gd_2 - g_1g_2)}{g} + 1 > 0$. Therefore, $H_{G'^3}(u, v') \geq H_{\tilde{G}^3}(u, v)$.

So the assertion holds. $\square$

Lemma 3.10. Let $\widehat{G}^3 \in \mathcal{U}_{n,d,g}$ be as above. Then $\varphi(U_{n,d,3}^*) > H_{\widehat{G}^3}(u, v)$.

Proof. Let $d_{\widehat{G}^3}(u, u_i) = d_1$, $d_{\widehat{G}^3}(u_j, v) = d_2$, $d_{\widehat{G}^3}(u_i, u_j) = g_1$ and $g - g_1 = g_2$. Since $d_{\widehat{G}^3}(u, u_i) + \lfloor \frac{g}{2} \rfloor = d$, $d_{\widehat{G}^3}(u_j, v) + \lfloor \frac{g}{2} \rfloor = d$ and $n \geq d_1 + d_2 + g$, similar to the computation of (10) and (11) in Lemma 3.6, we have

$$\varphi(U_{n,d,3}^*) - H_{\widehat{G}^3}(u, v) = 2 \left(d - d_1 - d_2 - \frac{g_1g_2}{g} \right) n - (d + d_1 + d_2 - 2)(d - d_1 - d_2)$$

$$\begin{aligned}
& +1 + 2gd_1 - 2g + \frac{2g_1g_2d_2}{g} + g_1g_2 \\
\geq & 2\left(d - d_1 - d_2 - \frac{g_1g_2}{g}\right)(d_1 + d_2 + g) \\
& - (d + d_1 + d_2 - 2)(d - d_1 - d_2) \\
& + 1 + 2gd_1 - 2g + \frac{2g_1g_2d_2}{g} + g_1g_2 \\
= & 2\left(2\left\lfloor\frac{g}{2}\right\rfloor - d - \frac{g_1g_2}{g}\right)\left(g + 2d - 2\left\lfloor\frac{g}{2}\right\rfloor\right) \\
& - \left(3d - 2\left\lfloor\frac{g}{2}\right\rfloor - 2\right)\left(2\left\lfloor\frac{g}{2}\right\rfloor - d\right) + 1 + 2gd \\
& - 2g\left\lfloor\frac{g}{2}\right\rfloor - 2g + g_1g_2 - \frac{2g_1g_2}{g}\left(d - \left\lfloor\frac{g}{2}\right\rfloor\right) \\
= & -d^2 + 4d\left\lfloor\frac{g}{2}\right\rfloor - \frac{6dg_1g_2}{g} - 2d + \frac{6g_1g_2\left\lfloor\frac{g}{2}\right\rfloor}{g} - 4\left\lfloor\frac{g}{2}\right\rfloor^2 \\
& + 2g\left\lfloor\frac{g}{2}\right\rfloor + 4\left\lfloor\frac{g}{2}\right\rfloor - 2g - g_1g_2 + 1.
\end{aligned}$$

Since $d > \left\lfloor\frac{g}{2}\right\rfloor$, $d_1 + d_2 + g_1 < d$, $1 \leq g_1 < 2\left\lfloor\frac{g}{2}\right\rfloor - d < \frac{g}{2}$, $g_1g_2 < (2\left\lfloor\frac{g}{2}\right\rfloor - d)(g - 2\left\lfloor\frac{g}{2}\right\rfloor + d)$, and by discussing the parity of g and computation, we have

$$\varphi(U_{n,d,3}^*) - H_{\widehat{G}^3}(u, v) > 0.$$

So the assertion holds. $\square$

Lemma 3.11. Let $G^{3*} \in \mathcal{U}_{n,g,d}$. If $u \in V(T_i^{3*})$ and $v \in V(T_j^{3*})$ be two pendant vertices of G^{3*} with $d_{G^{3*}}(u, v) < d$ and $d_{G^{3*}}(u, u_i) + \left\lfloor\frac{g}{2}\right\rfloor = d$ or $d_{G^{3*}}(u_j, v) + \left\lfloor\frac{g}{2}\right\rfloor = d$, then

$$\varphi(U_{n,d,3}^*) > H_{G^{3*}}(u, v).$$

Proof. Let $d_{G^{3*}}(u, u_i) = d_1$, $d_{G^{3*}}(u_j, v) = d_2$, $d_{G^{3*}}(u_i, u_j) = g_1$ and $g - g_1 = g_2$. Since $d_1 + \left\lfloor\frac{g}{2}\right\rfloor = d$ or $d_2 + \left\lfloor\frac{g}{2}\right\rfloor = d$, $n = d_1 + d_2 + g$, $d_1 + g_1 + d_2 < d$, $g_1 < d + g - n \leq \frac{g}{2}$, $g_1g_2 < (d + g - n)(n - d)$, similar to the computation of (10) and (11) in Lemma 3.6, we have

$$\begin{aligned}
\varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) &= 2(d - 1 - d_2)n - (d - 1)^2 + 2 + d_2^2 - d_1^2 - g_1g_2 - \frac{2g_1g_2d_1}{g} \\
&> d_2^2 - 2nd_2 + 2(d - 1)n - (d - 1)^2 + 2 - d_1^2 \\
&\quad - (d + g - n)(n - d)\frac{g + 2d_1}{g}.
\end{aligned}$$

Case 1. If $d_1 + \left\lfloor\frac{g}{2}\right\rfloor = d$ and $d_2 + \left\lfloor\frac{g}{2}\right\rfloor < d$, then $0 \leq d_2 = n - g - d + \left\lfloor\frac{g}{2}\right\rfloor \leq n - d - \frac{g}{2}$, $n \geq d + \frac{g}{2}$, and

$$\begin{aligned}
\varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) &\geq \left(n - d - \frac{g}{2}\right)^2 - 2n\left(n - d - \frac{g}{2}\right) + 2(d - 1)n - (d - 1)^2 + 2 - d_1^2 \\
&\quad - (d + g - n)(n - d)\frac{g + 2d_1}{g} \\
&= \frac{2d_1}{g}n^2 - \left(g + 2 + \frac{4d_1d}{g} + 2d_1\right)n - d_1^2
\end{aligned}$$

$$+2gd + \frac{g^2}{4} + (d+1)^2 + \frac{2d_1}{g}d^2 + 2d_1d.$$

Subcase 1.1. If g is even, $d_1 = d - \left\lfloor \frac{g}{2} \right\rfloor \geq 2$ and $n \geq d + \frac{g}{2}$, then $\frac{g}{2} \leq d - 2$ and

$$\begin{aligned} \varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) &\geq \frac{2d-g}{g} \left(d + \frac{g}{2}\right)^2 - \left(2 + \frac{4d^2}{g}\right) \left(d + \frac{g}{2}\right) + 2gd + (d+1)^2 + \frac{2d^3}{g} \\ &= \frac{3}{2}gd - \frac{g^2}{4} - g + 1 \\ &> 0. \end{aligned}$$

If g is even and $d_1 = d - \left\lfloor \frac{g}{2} \right\rfloor = 1$, then

$$\begin{aligned} \varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) &\geq \left(d - \frac{3}{2}\right)g + d + \frac{2d^2}{g} + \frac{2}{g} + 1 \\ &> 0. \end{aligned}$$

Subcase 1.2. If g is odd, then $\left\lfloor \frac{g}{2} \right\rfloor = \frac{g-1}{2}$, $n \geq d + \frac{g-1}{2}$. If $d_1 = d - \left\lfloor \frac{g}{2} \right\rfloor \geq 2$, then $\frac{g-1}{2} \leq d - 2$ and

$$\begin{aligned} \varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) &\geq -(2d+3)n - d_1^2 + 2gd + \frac{g^2}{4} + (d+1)^2 + 2d_1d \\ &> 0. \end{aligned}$$

If g is odd and $d_1 = d - \left\lfloor \frac{g}{2} \right\rfloor = 1$, then

$$\begin{aligned} \varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) &\geq -(2d+3)n - 1 + 2gd + \frac{g^2}{4} + (d+1)^2 + 2d \\ &> 0. \end{aligned}$$

Case 2. If $d_1 + \left\lfloor \frac{g}{2} \right\rfloor < d$ and $d_2 + \left\lfloor \frac{g}{2} \right\rfloor = d$, then $0 \leq d_1 = n - g - d + \left\lfloor \frac{g}{2} \right\rfloor \leq n - d - \frac{g}{2}$, $d + \frac{g}{2} \leq n < d + g$, and

$$\begin{aligned} \varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) &= 2\left(\left\lfloor \frac{g}{2} \right\rfloor - 1\right)n - (d-1)^2 \\ &\quad + 2 + (d_2 - d_1)(n - g) - g_1g_2 - \frac{2g_1g_2d_1}{g} \\ &= \left(g - n - \frac{2g_1g_2}{g}\right)d_1 + 2\left(\left\lfloor \frac{g}{2} \right\rfloor - 1\right)n \\ &\quad - (d-1)^2 + 2 + d_2(n - g) - g_1g_2 \\ &\geq \left(g - n - \frac{2g_1g_2}{g}\right)\left(n - d - \frac{g}{2}\right) + 2\left(\left\lfloor \frac{g}{2} \right\rfloor - 1\right)n \\ &\quad - (d-1)^2 + 2 + d_2(n - g) - g_1g_2. \end{aligned}$$

By discussing the parity of g and calculating as in Case 1, we have $\varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) > 0$.

Case 3. If $d_1 + \left\lfloor \frac{g}{2} \right\rfloor = d$ and $d_2 + \left\lfloor \frac{g}{2} \right\rfloor = d$, then we can refer to Lemma 3.10, and $\varphi(U_{n,d,3}^*) - H_{G^{3*}}(u, v) > 0$. $\square$

Lemma 3.12. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ with $|V(T_i)| \geq 2$. Let $S(G^3) = \{\widetilde{G}^3, \overline{G}^3, \widehat{G}^3\}$. If there exist two vertices $u \in V(T_i)$ and $v \in V(T_j)$ with $d_G(u, v) < d$ such that $\varphi(G) = H_G(u, v)$, then

$$\varphi(U_{n,d,3}^*) > \varphi(G).$$

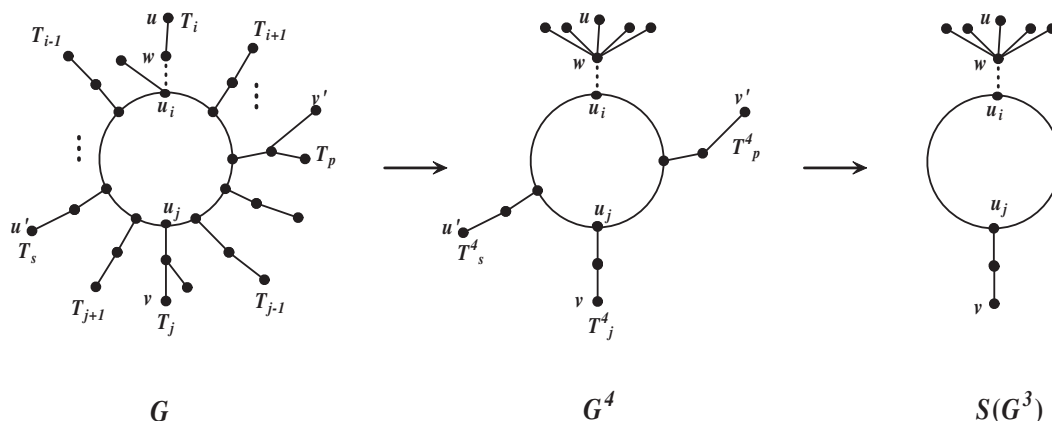


Figure 11: Transformation X

Proof. Since $G \in \mathcal{U}_{n,d,g}$, there exist two vertices such that the distance between these two vertices is d . Let w be the adjacent vertex of u in T_i . Then we need to consider the following cases.

Case 1. If there exist two vertices u' and v' in $V(G)$ such that $d_G(u', v') = d$, $u' \in V(T_s)$ and $v' \in V(T_p)$ with $s, p \neq i, j$, then $G^4 \in \mathcal{U}_{n,d,g}$ is a graph obtained from G by deleting all edges of T_r for all r with $r \neq i, j, s, p$, deleting all edges of T_s which do not belong to the $u_s u'$ -path, deleting all edges of T_p which do not belong to the $u_p v'$ -path, deleting all edges of T_i which do not belong to the $u_i u$ -path, deleting all edges of T_j which do not belong to the $u_j v$ -path, and adding these edges to the vertex w (see Figure 11). By repeating usage of Lemmas 3.1 and 3.5, we have $H_{G^4}(u, v) > H_G(u, v)$. Let $d_G(u, u_i) = d_1$ and $d_G(u_j, v) = d_2$. We consider the following cases.

Subcase 1.1. Let $G^4 = C(T_1^4, \dots, T_g^4) \in \mathcal{U}_{n,d,g}$. If there exists a vertex u_t on the cycle of G^4 with $d_{G^4}(u_t) = 2$ such that $d_{G^4}(u_t, u) = d$ and $d_{G^4}(u_j, v) + \lfloor \frac{g}{2} \rfloor < d$, then we can delete the all edges of T_s^4 and T_p^4 and add these edges to the vertex w , we get the new graph $\tilde{G}^3$ (see Figure 11). By repeating usage of Lemma 3.1, we have $H_{\tilde{G}^3}(u, v) > H_{G^4}(u, v)$. Next, if we delete a pendant edge of $\tilde{T}_i^3$ and insert a vertex in path $P_{u_j v}$ in $\tilde{T}_j^3$, then we get the new graph $\tilde{G}^{3'}$. Let $\tilde{G}^{3'} = C(\tilde{T}_1^{3'}, \dots, \tilde{T}_g^{3'})$.

If $d_{\tilde{G}^{3'}}(u, v) < d$, $d_{\tilde{G}^{3'}}(u_j, v) + \lfloor \frac{g}{2} \rfloor + 1 = d$ and $d_{\tilde{G}^{3'}}(u, u_i) + \lfloor \frac{g}{2} \rfloor = d$ in graph $\tilde{G}^{3'}$, then by Lemmas 3.1 and 3.10, we have

$$\varphi(U_{n,d,3}^*) > H_{\tilde{G}^{3'}}(u, v) \geq H_{\tilde{G}^3}(u, v) > H_{G^4}(u, v).$$

If $d_{\tilde{G}^{3'}}(u, v) = d$, then by Lemmas 3.1 and 3.6, we have

$$\varphi(U_{n,d,3}^*) > H_{\tilde{G}^{3'}}(u, v) \geq H_{\tilde{G}^3}(u, v) > H_{G^4}(u, v).$$

If $d_{\tilde{G}^{3'}}(u_j, v) + \lfloor \frac{g}{2} \rfloor + 1 < d$ and $d_{\tilde{G}^{3'}}(u, v) < d$, then we can continue to delete a pendant edge from $\tilde{T}_i^{3'}$ in $\tilde{G}^{3'}$ and insert a vertex to the path $P_{u_j v}$ in $\tilde{T}_j^{3'}$, repeating deleting edges and inserting vertices until that we get the new graph $\tilde{G} = C(\tilde{T}_1, \dots, \tilde{T}_g)$ such that $d_{\tilde{G}}(u, v) = d$ or there exist two vertices u_t and u_q on cycle with degree two such that $d_{\tilde{G}}(u, v) < d$ and $d_{\tilde{G}}(u_t, u) = d_{\tilde{G}}(u_q, v) = d$, or $\tilde{T}_i$ and $\tilde{T}_j$ are paths and there exist two vertices u_t and u_q on cycle with degree two such that $d_{\tilde{G}}(u, v) < d$ and $d_{\tilde{G}}(u_t, u) = d$ or $d_{\tilde{G}}(u_q, v) = d$, then by Lemmas 3.1, 3.6, 3.10 and 3.11, we have

$$\varphi(U_{n,d,3}^*) > H_{\tilde{G}}(u, v).$$

Subcase 1.2. If there exists a vertex u_t on the cycle of G^4 with $d(u_t) = 2$ such that $d_{G^4}(u_t, v) = d$ and $d_{G^4}(u, u_i) + \lfloor \frac{g}{2} \rfloor < d$, then we can delete the all edges of T_s^4 and T_p^4 and add these edges to the vertex w , we

get the new graph $\bar{G}^3$ (see Figure 11). By repeating usage of Lemma 3.1, we have $H_{\bar{G}^3}(u, v) > H_G(u, v)$. Next, if we delete a pendant edge of $\bar{T}_i^3$ and insert a vertex into the wu_i -path in $\bar{T}_i^3$, then we get the new graph $\bar{G}^{3'}$. Let $\bar{G}^{3'} = C(\bar{T}_1^{3'}, \dots, \bar{T}_g^{3'})$.

If $d_{\bar{G}^{3'}}(u, u_i) + \lfloor \frac{g}{2} \rfloor < d$ and $d_{\bar{G}^{3'}}(u, v) < d$, we can continue to repeat deleting pendant edges from $\bar{T}_i^{3'}$ and inserting vertices to wu_i -path in $\bar{T}_i^{3'}$ until that we get the new graph $\bar{G} = C(\bar{T}_1, \dots, \bar{T}_g)$ such that $d_{\bar{G}}(u, v) = d$ or there exist two vertices u_t and u_q on cycle with degree two such that $d_{\bar{G}}(u_q, u) = d_{\bar{G}}(u_t, v) = d$, or $\bar{T}_i$ and $\bar{T}_j$ are paths and there exist two vertices u_t and u_q on cycle with degree two such that $d_{\bar{G}}(u, v) < d$ and $d_{\bar{G}}(u_t, u) = d$ or $d_{\bar{G}}(u_q, v) = d$, then by Lemmas 3.1, 3.6, 3.10 and 3.11, we have

$$\varphi(U_{n,d,3}^*) > H_{\bar{G}}(u, v) > H_G(u, v).$$

Subcase 1.3. If there exist two vertices u_t and u_q on the cycle of G^4 with degree two such that $d_{G^4}(u_t, u) = d_{G^4}(u_q, v) = d$ and $d_{G^4}(u, v) < d$, then we can delete the all edges of T_s^4 and T_p^4 and add these edges to the vertex w , we get the new graph $\bar{G}^3$ (see Figure 11). By repeating usage of Lemmas 3.1 and 3.10, we have

$$\varphi(U_{n,d,3}^*) > H_{\bar{G}^3}(u, v) > H_G(u, v).$$

Subcase 1.4. If $d_{G^4}(u', u) = d$, $d_{G^4}(v', u) < d$, $d_{G^4}(u', v) < d$, $d_{G^4}(v', v) < d$ and there do not exist two vertices u_t and u_q on the cycle with degree two such that $d_{G^4}(u_t, u) = d$ and $d_{G^4}(u_q, v) = d$, then we can delete the all edges of T_p^4 and add these edges to the vertex w , we get the new graph G^5 . Then we can delete a pendant edge of T_s^5 in G^5 and insert a vertex into the wu_i -path of T_i^5 in G^5 , we denote this new graph as G^6 . If $d_{G^6}(u, v) < d$ and there does not exist a vertex u_t on the cycle such that $d_{G^6}(u_t, u) = d$, then we can continue to delete the pendant edge of T_s^6 and insert a vertex into the wu_i -path of T_i^6 in G^6 . By repeating deleting the pendant edge and inserting the edge until we get the graph $G^\#$ such that $d_{G^\#}(u, v) = d$ or there exists a vertex u_t on the cycle such that $d_{G^\#}(u_t, u) = d$. By the proof in **Subcase 1.1** and Lemmas 3.4, 3.6, we have

$$\varphi(U_{n,d,3}^*) > H_{G^\#}(u, v) > H_G(u, v).$$

Subcase 1.5. If $d_{G^4}(u', v) = d$, $d_{G^4}(u', u) < d$, $d_{G^4}(v', v) < d$, $d_{G^4}(v', u) < d$ and there do not exist two vertices u_t and u_q on the cycle with degree two such that $d_{G^4}(u_t, u) = d$ and $d_{G^4}(u_q, v) = d$, then we can delete the all edges of T_p^4 and add these edges to the vertex w , we get the new graph $\bar{G}^5$. Then we can delete a pendant edge of $\bar{T}_s^5$ in $\bar{G}^5$ and insert the edge to the u_jv -path of $\bar{T}_i^5$ in $\bar{G}^5$, we denote this new graph as $\bar{G}^6$. Let $\bar{G}^6 = C(\bar{T}_1^6, \dots, \bar{T}_g^6)$. By Theorem 2.1, we have

$$H_{\bar{G}^5}(u, v) = H_{\bar{G}^5}(u, u_i) + H_{\bar{G}^5}(u_i, u_j) + H_{\bar{G}^5}(u_j, v),$$

and

$$H_{\bar{G}^6}(u, v) = H_{\bar{G}^6}(u, u_i) + H_{\bar{G}^6}(u_i, u_j) + H_{\bar{G}^6}(u_j, v').$$

Let m_i be the number $\bar{T}_i^5$ and m_s be the number $\bar{T}_s^5$. Let $d_{\bar{G}^5}(u_j, v) = d_2$. Let G_1 and G_2 be two decomposed connected subgraphs of $\bar{G}^5$ through two vertices u_i and u_j such that G_1 contains $\bar{T}_i^5, \bar{T}_s^5$. Moreover, let $d_{G_1}(u_i, u_j) = g_1$, $d_{G_1}(u_s, u_j) = k_1$ and $d_{G_2}(u_i, u_j) = g_2$. By Theorems 2.2 and 2.3, we have

$$H_{\bar{G}^5}(u_i, u_j) = \frac{1}{g} (g_2(g_1^2 + 2m_i g_1 + 2m_s k_1) + g_1 g_2^2),$$

$$H_{\bar{G}^5}(u_j, v) = d_2^2 + 2(n - d_2)d_2.$$

Similarly, we have

$$H_{\bar{G}^6}(u_i, u_j) = \frac{1}{g} (g_2(g_1^2 + 2m_i g_1 + 2(m_s - 1)k_1) + g_1 g_2^2),$$

$$H_{\widetilde{G}^6}(u_j, v') = (d_2 + 1)^2 + 2(n - d_2 - 1)(d_2 + 1).$$

Since $H_{\widetilde{G}^5}(u, u_i) = H_{\widetilde{G}^6}(u, u_i)$, $m_i + m_s + g_1 + g_2 + d_2 = n$ and $g_1 > k_1$, we have

$$H_{\widetilde{G}^6}(u, v) - H_{\widetilde{G}^5}(u, v) = 2n - 2d_2 - 1 - \frac{2k_1g_2}{g} > 0.$$

If $d_{\widetilde{G}^6}(u, v) < d$ and there are not exist a vertex u_t on the cycle such that $d_{\widetilde{G}^6}(u_t, v) = d$, then we can continue to delete a pendant edge of $\widetilde{T}_s^6$ and insert a vertex to the u_jv -path of $\widetilde{T}_j^6$ in $\widetilde{G}^6$. By repeating deleting pendant edges and inserting vertices until we get the graph $G^\#$ such that $d_{G^\#}(u, v) = d$ or there exists a vertex u_t on the cycle such that $d_{G^\#}(u_t, v) = d$. By the proof in **Subcase 1.2** and Lemmas 3.4, 3.6, we have

$$\varphi(U_{n,d,3}^*) > H_{G^\#}(u, v) > H_{G^s}(u, v) > H_G(u, v).$$

Subcase 1.6. If $d_{G^4}(u', v) < d$, $d_{G^4}(u', u) < d$, $d_{G^4}(v', u) < d$, $d_{G^4}(v', v) < d$ and there do not exist two vertices u_t and u_q on the cycle with degree two such that $d_{G^4}(u_t, u) = d$, $d_{G^4}(u_q, v) = d$, then we can delete a pendant edge of T_i^4 in G^4 and insert a vertex into the wu_i -path of T_i^4 . We denote the new graph as $\widetilde{G}^5$. If $d_{\widetilde{G}^5}(u, v) < d$, $d_{\widetilde{G}^5}(u', v) < d$, $d_{\widetilde{G}^5}(u', u) < d$, $d_{\widetilde{G}^5}(v', u) < d$, $d_{\widetilde{G}^5}(v', v) < d$ and there do not exist two vertices u_t and u_q on the cycle with degree two such that $d_{\widetilde{G}^5}(u_t, u) = d$ and $d_{\widetilde{G}^5}(u_q, v) = d$, then we can continue to delete pendant edge of $\widetilde{T}_i^5$ and insert a vertex into the wu_i -path in $\widetilde{T}_i^5$, by repeating deleting pendant edges and inserting vertices until that we get the graph $G^\#$ such that $d_{G^\#}(u, v) = d$ or $d_{G^\#}(u, u') = d$ or $d_{G^\#}(u, v') = d$ or there exists a vertex u_t on the cycle such that $d_{G^\#}(u_t, u) = d$. By the discussions in above cases, we have

$$\varphi(U_{n,d,3}^*) > H_{G^\#}(u, v) > H_G(u, v).$$

Case 2. If there exists a vertex $u' \in V(T_p)$ such that $d_G(u', u) = d$, then $\widetilde{G}^4$ is the graph obtained from G by deleting all edges of T_r for all r with $r \neq i, j, p$, deleting all edges of T_p which do not belong to the u_pu' -path, deleting all edges of T_i which do not belong to the u_iu -path, deleting all edges of T_j which do not belong to the u_jv -path, and adding these edges to the vertex w . By repeating usage of Lemmas 3.1 and 3.5, we have $H_{\widetilde{G}^4}(u, v) > H_G(u, v)$. Next, similar to the graph transformation and the proof in **Subcase 1.4**, the assertion holds.

Case 3. If there exist a vertex $u' \in V(T_p)$ such that $d_G(u', v) = d$, then this case can refer to **Case 2** and **Subcase 1.5**. Similar to the graph transformation and the proof in **Subcase 1.5**, the assertion holds. $\square$

In Lemma 3.12, $\varphi(G) = H_G(u, v)$ and u is a pendant vertex. In the following lemma, we will discuss $\varphi(G) = H_G(u, v)$ and $d_G(u) = 2$, how the hitting time changes by graph transformation.

Lemma 3.13. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ and $n > g$. The number of pendant edges is larger than 3. If there exist two vertices u, v with $u \in V(T_i)$, $v \in V(T_j)$ such that $\varphi(G) = H_G(u, v)$ for $u = u_i$ and $d_G(u, v) < d$, G' is the graph obtained from G by deleting a pendant edge from pendant tree and adding it to the vertex u , the new added edge is $u'u$ (see Figure 12), then $H_{G'}(u', v) > H_G(u, v)$ and $\varphi(G') > \varphi(G)$.

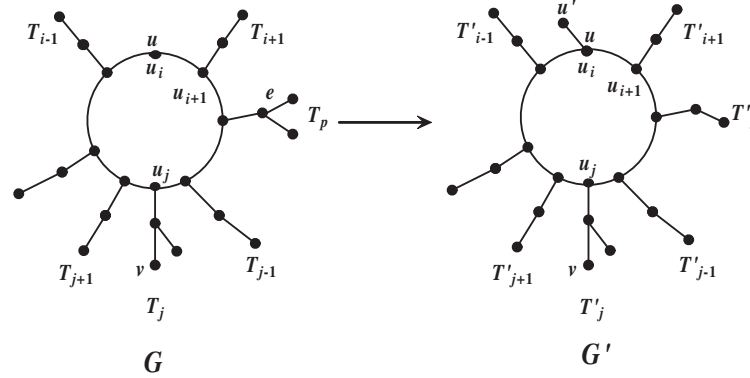


Figure 12: Transformation XI

Proof. Since $G \in \mathcal{U}_{n,d,g}$, there exist two vertices such that the distance between these two vertices is d . We need to consider the following cases.

Case 1. If $u^* \in V(T_r)$ and $v^* \in V(T_s)$ with $r, s \neq i, j$ such that $d_G(u^*, v^*) = d$, there do not exist a vertex w_1 such that $d_G(u, w_1) = d$, there do not exist a vertex w_2 such that $d_G(v, w_2) = d$, and there exists a tree T_p in G with $|V(T_p)| \geq 2$ or the number of pendant vertices of T_r (or T_s, T_j) is larger than 1, then we can get the new graph G' by deleting a pendant edge of T_p , or by deleting a pendant edge which does not incident with u^* (or v^*, v) of T_r (or T_s, T_j), and adding it to vertex u . The new added edge is $u'u$. By Lemma 3.1, we have $H_{G'}(u', v) > H_G(u, v)$ and $\varphi(G') > \varphi(G)$.

Case 2. If there exist vertices $v_1, v_2, \dots, v_k$ in $V(G)$ such that $d_G(v_i, u) = d$ for all i with $1 \leq i \leq k$, then we can get the new graph G' by deleting all the pendant edges incident with $v_1, v_2, \dots, v_k$ and adding these edges to vertex u . Let $u' \in V(T'_i)$ be a pendant vertex. By Lemma 3.1, we have $H_{G'}(u', v) > H_G(u, v)$ and $\varphi(G') > \varphi(G)$.

Case 3. If there exist vertices $v_1, v_2, \dots, v_t$ in $V(G)$ such that $d_G(v_i, v) = d$ for all i with $1 \leq i \leq k$ and there do not exist vertex u^* such that $d_G(u^*, u) = d$, and the number of pendant edges is larger than 2, then we can get the new graph G' by deleting the pendant edge of G and adding it to vertex u . If $t = 1$ and $v_1 \in V(T_p)$, then the deleted pendant edge is not the edge incident with v_1 and v . If $t \geq 2$, then the deleted pendant edge is not the edge incident with v . The new added edge is $u'u$. By Lemma 3.1, we have $H_{G'}(u', v) > H_G(u, v)$ and $\varphi(G') > \varphi(G)$. $\square$

In Lemma 3.13, when the number of pendant edges is larger than 3, we have discussed how the hitting time changes by graph transformation. The following corollary shows the result of the special cases that the pendant edge is not enough to perform the graph transformation.

Corollary 3.14. Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ and $n > g$. If the number of pendant edges is less than 4 and there exist two vertices u, v with $u \in V(T_i), v \in V(T_j)$ such that $\varphi(G) = H_G(u, v)$ for $u = u_i$ and $d_G(u, v) < d$, then we have the following results.

- (1) If $u^* \in V(T_r)$ and $v^* \in V(T_s)$ with $r, s \neq i, j$ such that $d_G(u^*, v^*) = d$, there do not exist a vertex w_1 such that $d_G(u, w_1) = d$, there do not exist a vertex w_2 such that $d_G(v, w_2) = d$, $|V(T_t)| = 1$ for all t with $t \neq j, r, s$, and T_j, T_r, T_s are paths, then $\varphi(U_{n,d,3}^*) \geq H_G(u, v)$.
- (2) If there exists only one vertex $v_1 \in V(T_p)$ such that $d_G(v_1, v) = d$, there do not exist vertex u^* such that $d_G(u^*, u) = d$, $|V(T_t)| = 1$ for all t with $t \neq j, p$, and T_p, T_j are paths, then $\varphi(U_{n,d,3}^*) \geq H_G(u, v)$.

Proof. Similar to the computation in Lemma 3.8, it is easy to get the result. $\square$

Remark: The above lemmas mainly discussed that $\varphi(G) = H_G(u, v)$ where vertices u and v belong to different pendant trees. We now turn to the case where both vertices are contained within the same pendant tree.

Lemma 3.15. *Let $G = C(T_1, \dots, T_g) \in \mathcal{U}_{n,d,g}$ with $n > g$. If there exist two vertices u, v with $u, v \in V(T_i)$ such that $\varphi(G) = H_G(u, v)$, then $\varphi(U_{n,d,3}^*) > \varphi(G)$.*

Proof. Since u and v lie in the same pendant tree T_i , the graph G decomposes into the path P_{uv} between u and v with its pendant branches. By Theorem 2.2, relocating any pendant edge to either u or its neighbor yields a modified graph G' satisfying $H_{G'}(u, v) \geq H_G(u, v)$. We perform this operation iteratively, moving edges to neighbor of u when $d(u, v) = d$, or to u otherwise. The operation will keep the diameter of the graph unchanged. This process produces an intermediate graph where the only pendant vertices are v and those adjacent to neighbor of u .

We proceed by cyclically reducing the graph: first decreasing the cycle length by 1 and applying the same edge relocation to obtain G'' with $H_{G''}(u, v) \geq H_G(u, v)$, repeating until achieving a 3-cycle. The cycle is then moved to neighbor of u , which Theorem 2.2 guarantees will increase $H_{G''}(u, v)$. Final application of the pendant edge relocation to any remaining branches yields the required extremal graph. $\square$

Now we are ready to present the proof of Theorem 1.1.

3.3. Proof of main Theorem

Proof of Theorem 1.1. While $\varphi(G) = H_G(u, v)$ and $d_G(u, v) = d$, by Lemmas 3.4, 3.5, 3.6, 3.8, we have $\varphi(U_{n,d,3}^*) > H_{G^3}(u, v) > H_G(u, v)$. While $\varphi(G) = H_G(u, v)$ and $d_G(u, v) < d$, if u is a pendant vertex, by Lemma 3.12, then $\varphi(U_{n,d,3}^*) > \varphi(G)$; if $d_G(u) = 2$, by Lemma 3.13 and Corollary 3.14, by graph transformation, this case can be transformed into the graph in Lemma 3.12. If u and v reside in the same tree, Lemma 3.15 provides the necessary conclusion. $\blacksquare$

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