

Peripheral Harary Index of Graphs

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Abstract In this paper, we introduce a new topological index for graphs called ‘Peripheral Harary Index’. The peripheral Harary index $PH(G)$ of a graph G is defined as the sum of the reciprocals of the distances between all unordered pairs of distinct peripheral vertices of G . We prove that $PH(G) = PH(G - v)$ and $PW(G) = PW(G - v)$, for any graph G with a pendant vertex v that is not in $P(G)$, where $PW(G)$ is the peripheral Wiener index. We compute $PH(G)$, obtain some bounds for some standard graphs and graph operations. Further, we establish a formula for computation of $PH(G)$ and present an algorithm for its computation using adjacency matrix.

1 Introduction

For standard terminology and notion in graph theory, we follow the text-book of Harary [5]. The non-standard ones will be given in this paper as and when required.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The distance between two vertices u and v in G , denoted by $d_G(u, v)$ (or simply $d(u, v)$) is the number of edges in a shortest path (also called a graph geodesic) connecting them. We write $u \sim v$ to denote two vertices u and v are adjacent in G .

The eccentricity of a vertex v in G , denoted by $e_G(v)$ (or simply $e(v)$), is the maximum distance between v and any other vertex in G . The maximum eccentricity of all the vertices in G is called the diameter of G and is denoted by $d(G)$. A vertex with maximum eccentricity in G is called a peripheral vertex in G . So, vertices whose eccentricities are equal to diameter of G are the peripheral vertices of G . The set of all peripheral vertices of G is denoted by $P(G)$.

If $P(G) = V(G)$, then G is called a peripheral graph (self-centered graph). The pair $\{u, v\}$ denotes the unordered pair of vertices u, v with $u \neq v$. A vertex with minimum eccentricity in G is called a center of G . The set of all center vertices of G is denoted by $C(G)$. A graph G is almost self-centered if every vertex in G is a center except for two. A graph G is almost peripheral if every vertex in G is a peripheral vertex except for one (the exceptional vertex is nothing but the center of G).

Wiener index, Harary index (Reciprocal Wiener index), and peripheral Wiener index are some important distance based topological indices defined for graphs having applications in Chemistry (see [3], [6], [8], [10], [11], [12] and [13]). The Wiener index $W(G)$ of a graph G is

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defined as

$$W(G) = \sum_{\{u,v\} \subset V(G)} d(u,v) \quad (1.1)$$

The Harary index (or Reciprocal Wiener index) $H(G)$ of a graph G is defined as

$$H(G) = \sum_{\{u,v\} \subset V(G)} \frac{1}{d(u,v)} \quad (1.2)$$

The peripheral Wiener index $PW(G)$ (see [10]) of a graph G is defined as

$$PW(G) = \sum_{\{u,v\} \subset P(G)} d(u,v) \quad (1.3)$$

Motivated by the above mentioned indices, we introduce a new topological index called the peripheral Harary index. The peripheral Harary index $PH(G)$ of a graph G is defined as the sum of the reciprocals of the distances between all unordered pairs of distinct peripheral vertices of G . In section 2, we give an example and make some observations. In section 3, we present some important results on computing $PH(G)$, obtain some bounds for some standard graphs and graph operations. In section 4, we establish a formula for computation of $PH(G)$ and present an algorithm for its computation using adjacency matrix. In Theorem 3.1, we prove that $PH(G) = PH(G - v)$ and $PW(G) = PW(G - v)$, for any graph G with a pendant vertex v that is not in $P(G)$. The graphs considered in this paper are all connected graphs with at least two vertices.

2 Definition, Example and Observations

Definition 2.1. The peripheral Harary index $PH(G)$ of a graph G is defined as

$$PH(G) = \sum_{\{u,v\} \subset P(G)} \frac{1}{d(u,v)} \quad (2.1)$$

Example 2.2. We compute the peripheral Harary index of the hydrogen-depleted molecular graph G of 1-Ethyl-2-methylcyclobutane C_7H_{14} . We label the vertices of G as shown in Figure 1.

Here, $P(G) = \{a, f, h\}$. We have $d(a, f) = 4$, $d(a, h) = 2$, and $d(f, h) = 4$. The peripheral Harary index of G is

$$\begin{aligned} PH(G) &= \frac{1}{d(a, f)} + \frac{1}{d(a, h)} + \frac{1}{d(f, h)} \\ &= \frac{1}{4} + \frac{1}{2} + \frac{1}{4} \\ &= 1. \end{aligned}$$

Observations:

- (i) If there are k peripheral vertices in a graph G , then we have $\binom{k}{2}$ unordered pairs of distinct peripheral vertices in G and for any pair $\{u, v\} \subset P(G)$, $1 \leq d(u, v) \leq d(G)$. Hence from (2.1), we have,

$$\frac{1}{d(G)} \binom{k}{2} \leq PH(G) \leq \binom{k}{2}.$$

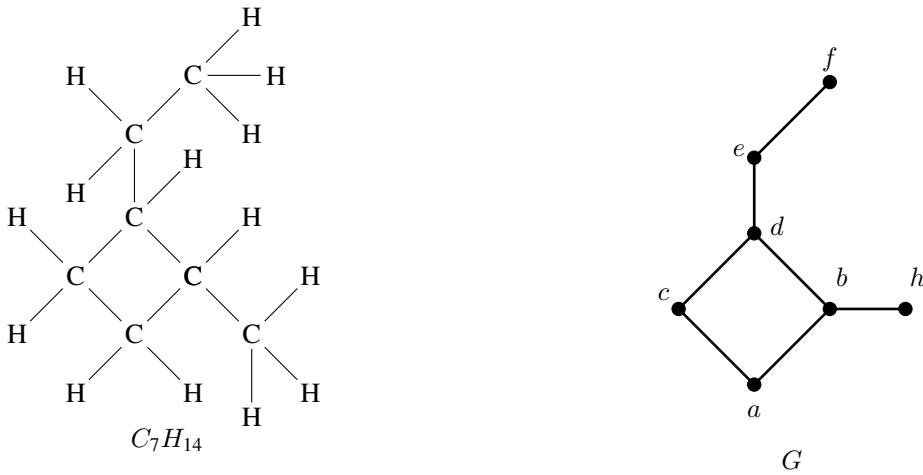


Figure 1. 1-Ethyl-2-methylcyclobutane C_7H_{14} and the corresponding hydrogen-depleted molecular graph G

(ii) In any graph G , $P(G) \subseteq V(G)$. Therefore,

$$PH(G) \leq H(G)$$

and it is easy to see that

$$PH(G) = H(G) \iff G \text{ is a peripheral graph.}$$

(iii) For any graph G with k peripheral vertices, by AM-HM inequality, we have,

$$PW(G) \cdot PH(G) \geq \binom{k}{2}^2.$$

(iv) For an almost self-centered graph G ,

$$PH(G) = \frac{1}{d(G)}.$$

(v) For a graph G ,

$$PH(G) = H(G) - \sum_{\substack{u \in P(G), \\ v \in V(G) - P(G)}} \frac{1}{d(u, v)} - \sum_{\{u, v\} \in V(G) - P(G)} \frac{1}{d(u, v)} \tag{2.2}$$

(vi) For an almost peripheral graph G with (unique) central vertex c ,

$$PH(G) = H(G) - \sum_{v \in V(G) - \{c\}} \frac{1}{d(c, v)}.$$

(vii) For a graph G of diameter 2 with n vertices and $k \geq 2$ vertices of eccentricity 1, from (2.2), it follows that,

$$PH(G) = H(G) - k(n - k) - \binom{k}{2}.$$

3 Some Important Results

Theorem 3.1. *Let G be a graph and v be a pendant vertex that is not in $P(G)$. Then $PH(G) = PH(G - v)$ and $PW(G) = PW(G - v)$.*

Proof. Since $v \notin P(G)$ and v is a pendant vertex, it follows that, $e_G(u) = e_{G-v}(u)$, $\forall u \in V(G - v)$ and $e_G(v) < d(G)$. Hence

$$\begin{aligned} d(G) &= \max\{e_G(u) : u \in V(G) - \{v\}\} \\ &= \max\{e_{G-v}(u) : u \in V(G - v)\} \\ &= d(G - v). \end{aligned}$$

We claim that $P(G) = P(G - v)$. Let $u \in P(G - v)$. Then $e_{G-v}(u) = d(G - v) = d(G)$. Hence $u \in P(G)$. So $P(G - v) \subseteq P(G)$. Suppose that $u \in P(G)$. Then $e_G(u) = d(G) = d(G - v)$, where $u \neq v$ by assumption. Hence $u \in P(G - v)$. So $P(G - v) \subseteq P(G)$. This proves the claim and hence the result. \square

From the Theorem 3.1, the following corollary is immediate.

Corollary 3.2. *Let G be a graph and S be the set of all pendant vertices which are not in $P(G)$. Then $PH(G) = PH(G - S)$ and $PW(G) = PW(G - S)$, where $G - S$ denotes the graph obtained from G by removing all the vertices in S .*

Proposition 3.3. *For the wheel graph W_n on $n \geq 4$ vertices,*

$$PH(W_n) = \begin{cases} 6, & \text{if } n = 4; \\ (n - 1)(n - 3), & \text{if } n \geq 5. \end{cases}$$

Proof. We have $W_4 = K_4$, and so $PH(W_4) = H(W_4) = 6$.

In W_n , $n \geq 5$, there are $n - 1$ peripheral vertices. Let v be a peripheral vertex. There are exactly 2 peripheral vertices adjacent to v and there are exactly $n - 1 - 1 - 2 = n - 4$ vertices at distance 2 from v . Therefore the sum of distances from v to other peripheral vertices is $1 \cdot 2 + 2 \cdot (n - 4) = 2(n - 3)$. Since there are $n - 1$ peripheral vertices,

$$PH(W_n) = \frac{1}{2} \cdot 2(n - 1)(n - 3) = (n - 1)(n - 3). \quad \square$$

Proposition 3.4. *Let $Wd(n, m)$ denotes the windmill graph constructed for $n \geq 2$ and $m \geq 2$ by joining m copies of the complete graph K_n at a shared common vertex v . Then we have*

$$PH(Wd(n, m)) = \frac{m(n - 1)(n - 2)}{2} + \frac{m(m - 1)(n - 1)^2}{4}.$$

Hence,

(i) *for the friendship graph F_k on $2k + 1$ vertices,*

$$PH(F_k) = k^2;$$

(ii) *for the star $K_{1,n}$ on $n + 1$ vertices,*

$$PH(K_{1,n}) = \frac{n(n - 1)}{4}.$$

Proof. Clearly, the diameter of $Wd(n, m)$ is 2 and $P(Wd(n, m)) = V - \{v\}$. Let H_1, \dots, H_m be the components of $Wd(n, m) - v$. Note that $H_i \cong K_{n-1}$, $\forall i$ and for any $u, v \in P(Wd(n, m))$, $u \neq v$, we have

$$d(u, v) = \begin{cases} 1, & \text{if } \{u, v\} \subset V(H_i) \text{ for some } i, 1 \leq i \leq m; \\ 2, & \text{if } u \in V(H_i), v \in V(H_j), 1 \leq i < j \leq m \end{cases}$$

Hence from (2.1), we have

$$\begin{aligned} PH(Wd(n, m)) &= \sum_{\{u,v\} \subset P(Wd(n,m))} \frac{1}{d(u,v)} \\ &= \sum_{\substack{\{u,v\} \subset V(H_i), \\ 1 \leq i \leq m}} \frac{1}{1} + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq m}} \frac{1}{2} \\ &= m \binom{n-1}{2} + \frac{1}{2} \cdot \frac{1}{2} m(n-1)(n-1)(m-1) \\ &= \frac{m(n-1)(n-2)}{2} + \frac{m(m-1)(n-1)^2}{4}. \end{aligned} \quad (3.1)$$

Since the friendship graph F_k on $2k + 1$ vertices is nothing but $Wd(3, k)$, it follows from (3.1) that

$$\begin{aligned} PH(F_k) &= \frac{k(3-1)(3-2)}{2} + \frac{k(k-1)(3-1)^2}{4} \\ &= k^2. \end{aligned}$$

Since the star $K_{1,n}$ on $n + 1$ vertices is nothing but $Wd(2, n)$, it follows from (3.1) that

$$\begin{aligned} PH(F_k) &= \frac{n(2-1)(2-2)}{2} + \frac{n(n-1)(2-1)^2}{4} \\ &= \frac{n(n-1)}{4}. \end{aligned} \quad \square$$

Proposition 3.5. Let G be the corona product $K_m \circ K_n$ of complete graphs K_m and K_n where $m \geq 2$ and $n \geq 1$. Then we have

$$PH(G) = \frac{mn(n-1)}{2} + \frac{m(m-1)n^2}{6}.$$

Proof. The set of peripheral vertices of G , $P(G) = V(G) - V(K_m)$ (that is all vertices of G lying in the different copies of K_n). Let H_1, \dots, H_m be the components of $G - V(K_m)$ (that is the graph obtained from G by deleting the vertices of the copy of K_m). Note that $H_i \cong K_n$, $\forall i$ and for any $u, v \in P(G)$, $u \neq v$, we have,

$$d(u, v) = \begin{cases} 1, & \text{if } \{u, v\} \subset V(H_i) \text{ for some } i, 1 \leq i \leq m; \\ 3, & \text{if } u \in V(H_i), v \in V(H_j), 1 \leq i < j \leq m \end{cases}$$

Hence from (2.1), we have

$$PH(G) = \sum_{\{u,v\} \subset P(G)} \frac{1}{d(u,v)}$$

$$\begin{aligned}
 &= \sum_{\substack{\{u,v\} \subset V(H_i), \\ 1 \leq i \leq m}} \frac{1}{1} + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq m}} \frac{1}{3} \\
 &= \frac{mn(n-1)}{2} + \frac{m(m-1)n^2}{6}. \quad \square
 \end{aligned}$$

Proposition 3.6. *Let G be a graph with $m \geq 2$ vertices. Let G' be the corona product $G \circ K_n$ of G and the complete graph K_n , $n \geq 1$. Then*

$$\frac{kn(n-1)}{2} + \frac{k(k-1)n^2}{2(d(G)+2)} \leq PH(G') \leq \frac{kn(n-1)}{2} + \frac{k(k-1)n^2}{6},$$

where $k = |P(G)|$.

Proof. Let H_1, \dots, H_m be the components of $G' - V(G)$. Note that $H_i \cong K_n, \forall i$. Let v_1, \dots, v_k be the peripheral vertices of G . Then, clearly $P(G') = \cup_{i=1}^k V(H_i)$. Now, for $\{u, v\} \subset V(H_i), 1 \leq i \leq k$, we have, $d(u, v) = 1$, and for $u \in V(H_i), v \in V(H_j), i \neq j$, we have

$$3 \leq d_{G'}(u, v) \leq d(G) + 2 \tag{3.2}$$

Hence from (2.1), we have

$$\begin{aligned}
 PH(G') &= \sum_{\{u,v\} \subset P(G')} \frac{1}{d(u,v)} \\
 &= \sum_{\substack{\{u,v\} \subset V(H_i), \\ 1 \leq i \leq k}} \frac{1}{1} + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u,v)} \\
 &= k \frac{n(n-1)}{2} + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u,v)} \tag{3.3}
 \end{aligned}$$

From (3.2), we have

$$\sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d(G)+2} \leq \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u,v)} \leq \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{3},$$

that is

$$\frac{k(k-1)n^2}{2(d(G)+2)} \leq \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u,v)} \leq \frac{k(k-1)n^2}{6} \tag{3.4}$$

Using (3.4) in (3.3), we have

$$\frac{kn(n-1)}{2} + \frac{k(k-1)n^2}{2(d(G)+2)} \leq PH(G') \leq \frac{kn(n-1)}{2} + \frac{k(k-1)n^2}{6}. \quad \square$$

Proposition 3.7. *Let $G = (V, E)$ be a graph with $n \geq 1$ vertices. Let G' be the corona product $K_m \circ G$ of the complete graph $K_m, m \geq 2$ and G . Then*

$$PH(G) = \frac{m}{2}|E| + \frac{mn(n-1)}{4} + \frac{m(m-1)n^2}{6}.$$

Proof. The set of peripheral vertices of G' , $P(G') = V(G') - V(K_m)$. Let H_1, \dots, H_m be the components of $G' - V(K_m)$. Note that $H_i \cong G$, $\forall i$ and for any $u, v \in P(G')$, $u \neq v$, we have,

$$d_{G'}(u, v) = \begin{cases} 1, & \text{if } \{u, v\} \subset V(H_i) \text{ for some } i, 1 \leq i \leq m \text{ and } u \sim v; \\ 2, & \text{if } \{u, v\} \subset V(H_i) \text{ for some } i, 1 \leq i \leq m \text{ and } u \not\sim v; \\ 3, & \text{if } u \in V(H_i), v \in V(H_j), 1 \leq i < j \leq m. \end{cases}$$

Hence from (2.1), we have

$$\begin{aligned} PH(G') &= \sum_{\{u,v\} \subset P(G')} \frac{1}{d_{G'}(u,v)} \\ &= \sum_{\substack{\{u,v\} \subset V(H_i), \\ 1 \leq i \leq m \\ u \sim v}} \frac{1}{1} + \sum_{\substack{\{u,v\} \subset V(H_i), \\ 1 \leq i \leq m \\ u \not\sim v}} \frac{1}{2} + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq m}} \frac{1}{3} \\ &= m|E| + \frac{1}{2}m \left[\frac{n(n-1)}{2} - |E| \right] + \frac{m(m-1)n^2}{6} \\ &= \frac{m}{2}|E| + \frac{mn(n-1)}{4} + \frac{m(m-1)n^2}{6}. \end{aligned} \quad \square$$

Proposition 3.8. *Let G be a graph with $m \geq 2$ vertices and H be a graph with $n \geq 1$ vertices. Let G' be the corona product $G \circ H$ of the graphs G and H . Then*

$$\begin{aligned} \frac{k}{2}|E(H)| + \frac{kn(n-1)}{4} + \frac{k(k-1)n^2}{2(d(G)+2)} \\ \leq PH(G') \leq \frac{k}{2}|E(H)| + \frac{kn(n-1)}{4} + \frac{k(k-1)n^2}{6}, \end{aligned}$$

where $k = |P(G)|$.

Proof. Let H_1, \dots, H_m be the components of $G' - V(G)$. Note that $H_i \cong H$, $\forall i$. Let v_1, \dots, v_k be the peripheral vertices of G . Then, clearly $P(G') = \cup_{i=1}^k V(H_i)$. Now, for any $u, v \in P(G')$, $u \neq v$, we have

$$d_{G'}(u, v) = \begin{cases} 1, & \text{if } \{u, v\} \subset V(H_i) \text{ for some } i, 1 \leq i \leq k \text{ and } u \sim v; \\ 2, & \text{if } \{u, v\} \subset V(H_i) \text{ for some } i, 1 \leq i \leq k \text{ and } u \not\sim v, \end{cases}$$

and for $u \in V(H_i), v \in V(H_j), 1 \leq i < j \leq k$, we have

$$3 \leq d_{G'}(u, v) \leq d(G) + 2 \tag{3.5}$$

Hence from (2.1), we have

$$\begin{aligned} PH(G') &= \sum_{\{u,v\} \subset P(G')} \frac{1}{d_{G'}(u,v)} \\ &= \sum_{\substack{\{u,v\} \subset V(H_i), \\ 1 \leq i \leq k \\ u \sim v}} \frac{1}{1} + \sum_{\substack{\{u,v\} \subset V(H_i), \\ 1 \leq i \leq k \\ u \not\sim v}} \frac{1}{2} + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u,v)} \end{aligned}$$

$$\begin{aligned}
 &= k|E(H)| + \frac{1}{2}k \left[\frac{n(n-1)}{2} - |E(H)| \right] + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u, v)} \\
 &= \frac{k}{2}|E(H)| + \frac{kn(n-1)}{4} + \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u, v)} \tag{3.6}
 \end{aligned}$$

From (3.5), we have

$$\sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d(G) + 2} \leq \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u, v)} \leq \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{3},$$

that is

$$\frac{k(k-1)n^2}{2(d(G) + 2)} \leq \sum_{\substack{u \in V(H_i), v \in V(H_j), \\ 1 \leq i < j \leq k}} \frac{1}{d_{G'}(u, v)} \leq \frac{k(k-1)n^2}{6} \tag{3.7}$$

Using (3.7) in (3.6), we have

$$\begin{aligned}
 \frac{k}{2}|E(H)| + \frac{kn(n-1)}{4} + \frac{k(k-1)n^2}{2(d(G) + 2)} \\
 \leq PH(G') \leq \frac{k}{2}|E(H)| + \frac{kn(n-1)}{4} + \frac{k(k-1)n^2}{6}. \quad \square
 \end{aligned}$$

Proposition 3.9. For the $m \times n$ grid graph $P_m \times P_n$ (the graph Cartesian product of path graphs on $m \geq 2$ and $n \geq 2$ vertices),

$$PH(P_m \times P_n) = 2 \left(\frac{1}{m-1} + \frac{1}{n-1} + \frac{1}{m+n-2} \right).$$

Hence, for the ladder graph $P_n \times P_2$,

$$PH(P_n \times P_2) = 2 \left(\frac{1}{n-1} + \frac{1}{n} + 1 \right).$$

Proof. In the grid graph $P_m \times P_n$, there are exactly 4 peripheral vertices each of eccentricity $m + n$, situated at the four corners of the grid. Let v_1, v_2, v_3 and v_4 be the peripheral vertices $P_m \times P_n$. Therefore from (2.1), we have

$$\begin{aligned}
 PH(P_m \times P_n) &= \sum_{1 \leq i < j \leq 4} \frac{1}{d(v_i, v_j)} \\
 &= 2 \left(\frac{1}{m-1} + \frac{1}{n-1} + \frac{1}{m+n-2} \right) \tag{3.8}
 \end{aligned}$$

From (3.8), for the ladder graph $P_n \times P_2$, it follows that,

$$\begin{aligned}
 PH(P_n \times P_2) &= 2 \left(\frac{1}{n-1} + \frac{1}{2-1} + \frac{1}{n+2-2} \right) \\
 &= 2 \left(\frac{1}{n-1} + \frac{1}{n} + 1 \right). \quad \square
 \end{aligned}$$

Proposition 3.10. *Let $G = P_m \times C_n$ denote the cylinder graph with $m \geq 2$ and $n \geq 3$. Then*

$$PH(G) = 2PH(C_n) + nPH(P_m) + 2n \left(\frac{1}{m} + \frac{1}{m+1} + \dots + \frac{1}{m + \lfloor \frac{n}{2} \rfloor - 2} \right) + \frac{n2^{\epsilon(n)}}{m + \lfloor \frac{n}{2} \rfloor - 1},$$

where $\epsilon(n) = \begin{cases} 0 & \text{when } n \text{ is even;} \\ 1 & \text{when } n \text{ is odd.} \end{cases}$

Proof. We have

$$PH(C_n) = H(C_n) = \frac{n}{2} \left[2 \left(1 + \frac{1}{2} + \dots + \frac{1}{\lfloor \frac{n}{2} \rfloor - 1} \right) + \frac{2^{\epsilon(n)}}{\lfloor \frac{n}{2} \rfloor} \right] \tag{3.9}$$

and

$$PH(P_m) = \frac{1}{d(P_m)} = \frac{1}{m-1} \tag{3.10}$$

Clearly, the number of peripheral vertices in G is $2n$. For any $v \in P(G)$, we have

$$\begin{aligned} & \sum_{u \in P(G) - \{v\}} \frac{1}{d_G(u, v)} \\ &= 2 \left(1 + \frac{1}{2} + \dots + \frac{1}{\lfloor \frac{n}{2} \rfloor - 1} \right) + \frac{2^{\epsilon(n)}}{\lfloor \frac{n}{2} \rfloor} + \frac{1}{m-1} \\ &+ 2 \left(\frac{1}{(m-1)+1} + \frac{1}{(m-1)+2} + \dots + \frac{1}{(m-1) + \lfloor \frac{n}{2} \rfloor - 1} \right) \\ &+ \frac{2^{\epsilon(n)}}{(m-1) + \lfloor \frac{n}{2} \rfloor}. \end{aligned}$$

Hence,

$$\begin{aligned} PH(G) &= \frac{1}{2} \sum_{v \in P(G)} \sum_{u \in P(G) - \{v\}} \frac{1}{d_G(u, v)} \\ &= n \left[2 \left(1 + \frac{1}{2} + \dots + \frac{1}{\lfloor \frac{n}{2} \rfloor - 1} \right) + \frac{2^{\epsilon(n)}}{\lfloor \frac{n}{2} \rfloor} \right] + \frac{n}{m-1} \\ &+ 2n \left(\frac{1}{(m-1)+1} + \frac{1}{(m-1)+2} + \dots + \frac{1}{(m-1) + \lfloor \frac{n}{2} \rfloor - 1} \right) \\ &+ \frac{n2^{\epsilon(n)}}{(m-1) + \lfloor \frac{n}{2} \rfloor} \\ &= 2PH(C_n) + nPH(P_m) + 2n \left(\frac{1}{m} + \frac{1}{m+1} + \dots + \frac{1}{m + \lfloor \frac{n}{2} \rfloor - 2} \right) \\ &+ \frac{n2^{\epsilon(n)}}{m + \lfloor \frac{n}{2} \rfloor - 1} \quad \text{(using (3.9) and (3.10)).} \end{aligned}$$

□

We use the following two lemmas (see [7]) to discuss the computation of Peripheral Harary index for the Cartesian product of graphs.

Lemma 3.11. [7] *Let G and H be graphs, and let $(g, h), (g', h')$ be vertices of $G \times H$. Then*

$$d_{G \times H}((g, h), (g', h')) = d_G(g, g') + d_H(h, h').$$

Lemma 3.12. [7] *For two graphs G_1 and G_2 ,*

$$P(G_1 \times G_2) = P(G_1) \times P(G_2).$$

Theorem 3.13. *For two graphs G_1 and G_2 with k_1 and k_2 peripheral vertices respectively,*

$$\begin{aligned} k_2 PH(G_1) + k_1 PH(G_2) + \frac{1}{d(G_1) + d(G_2)} \binom{k_1}{2} \binom{k_2}{2} \\ \leq PH(G_1 \times G_2) \leq k_2 PH(G_1) + k_1 PH(G_2) + \frac{1}{2} \binom{k_1}{2} \binom{k_2}{2}. \end{aligned}$$

Proof. Let $P(G_1) = \{u_1, \dots, u_{k_1}\}$ and $P(G_2) = \{v_1, \dots, v_{k_2}\}$. From (2.1), we write

$$PH(G_1) = \sum_{1 \leq i < j \leq k_1} \frac{1}{d_{G_1}(u_i, u_j)} \tag{3.11}$$

and

$$PH(G_2) = \sum_{1 \leq i < j \leq k_2} \frac{1}{d_{G_2}(v_i, v_j)} \tag{3.12}$$

By Lemma 3.12 and using (2.1), we have

$$\begin{aligned} PH(G_1 \times G_2) &= \sum_{\substack{1 \leq i, j \leq k_1, 1 \leq k, l \leq k_2, \\ i \neq j \text{ or } k \neq l}} \frac{1}{d_{G_1 \times G_2}((u_i, v_k), (u_j, v_l))} \\ &= \sum_{\substack{1 \leq i, j \leq k_1, 1 \leq k, l \leq k_2, \\ i \neq j \text{ or } k \neq l}} \frac{1}{d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l)} \quad (\text{from Lemma 3.11}) \\ &= \sum_{\substack{1 \leq i < j \leq k_1, \\ 1 \leq k = l \leq k_2}} \frac{1}{d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l)} \\ &\quad + \sum_{\substack{1 \leq i = j \leq k_1, \\ 1 \leq k < l \leq k_2}} \frac{1}{d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l)} \\ &\quad + \sum_{\substack{1 \leq i < j \leq k_1, \\ 1 \leq k < l \leq k_2}} \frac{1}{d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l)} \\ &= k_2 PH(G_1) + k_1 PH(G_2) + \sum_{\substack{1 \leq i < j \leq k_1, \\ 1 \leq k < l \leq k_2}} \frac{1}{d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l)} \tag{3.13} \end{aligned}$$

Now, for any $1 \leq i < j \leq k_1$ and $1 \leq k < l \leq k_2$, we have

$$2 \leq d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l) \leq d(G_1) + d(G_2)$$

which implies

$$\sum_{\substack{1 \leq i < j \leq k_1, \\ 1 \leq k < l \leq k_2}} \frac{1}{d(G_1) + d(G_2)} \leq \sum_{\substack{1 \leq i < j \leq k_1, \\ 1 \leq k < l \leq k_2}} \frac{1}{d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l)} \leq \sum_{\substack{1 \leq i < j \leq k_1, \\ 1 \leq k < l \leq k_2}} \frac{1}{2}$$

that is

$$\frac{1}{d(G_1) + d(G_2)} \binom{k_1}{2} \binom{k_2}{2} \leq \sum_{\substack{1 \leq i < j \leq k_1, \\ 1 \leq k < l \leq k_2}} \frac{1}{d_{G_1}(u_i, u_j) + d_{G_2}(v_k, v_l)} \leq \frac{1}{2} \binom{k_1}{2} \binom{k_2}{2} \tag{3.14}$$

Using (3.14) in (3.13), we get

$$\begin{aligned} k_2 PH(G_1) + k_1 PH(G_2) + \frac{1}{d(G_1) + d(G_2)} \binom{k_1}{2} \binom{k_2}{2} \\ \leq PH(G_1 \times G_2) \leq k_2 PH(G_1) + k_1 PH(G_2) + \frac{1}{2} \binom{k_1}{2} \binom{k_2}{2}. \end{aligned} \quad \square$$

The following Corollary is immediate from Theorem 3.13.

Corollary 3.14. For a graph G with k peripheral vertices,

$$2k PH(G) + \frac{1}{2d(G)} \binom{k}{2}^2 \leq PH(G \times G) \leq 2k PH(G) + \frac{1}{2} \binom{k}{2}^2.$$

Proposition 3.15. Let $G = T_{\Delta}^k$ denote the Dendrimer tree (see [14]), which is a rooted tree with level k where every non-pendent vertex is of degree Δ . Then

$$PH(G) = \begin{cases} \frac{\Delta(\Delta-1)}{4}, & \text{for } k = 1; \\ \frac{\Delta(\Delta-1)(\Delta-2)}{4} + \frac{\Delta(\Delta-1)^2}{8}, & \text{for } k = 2; \\ \frac{\Delta(\Delta-1)^{k-1}}{4} \left[(\Delta-1) \left\{ 1 + \frac{1}{2} + \dots + \frac{1}{k-1} + \frac{(\Delta-1)^{k-1}}{k} \right\} - 1 \right], & \text{for } k \geq 3. \end{cases}$$

Proof. Clearly the number of peripheral vertices in G is $\Delta(\Delta-1)^{k-1}$. For any $v \in P(G)$, we have

$$\sum_{u \in P(G) - \{v\}} \frac{1}{d_G(u, v)} = \begin{cases} \frac{(\Delta-1)}{2}, & \text{for } k = 1; \\ \frac{(\Delta-2)}{2} + \frac{(\Delta-1)^2}{4}, & \text{for } k = 2 \end{cases}$$

and for $k \geq 3$,

$$\begin{aligned} \sum_{u \in P(G) - \{v\}} \frac{1}{d_G(u, v)} &= \frac{(\Delta-2)}{2} + \frac{(\Delta-1)}{4} + \dots + \frac{(\Delta-1)}{2(k-1)} + \frac{(\Delta-1)^k}{2k} \\ &= \frac{(\Delta-1)}{2} \left\{ 1 + \frac{1}{2} + \dots + \frac{1}{k-1} + \frac{(\Delta-1)^{k-1}}{k} \right\} - \frac{1}{2}. \end{aligned}$$

Hence

$$\begin{aligned} PH(G) &= \frac{1}{2} \sum_{v \in P(G)} \sum_{u \in P(G) - \{v\}} \frac{1}{d_G(u, v)} \\ &= \begin{cases} \frac{\Delta(\Delta-1)}{4}, & \text{for } k = 1; \\ \frac{\Delta(\Delta-1)(\Delta-2)}{4} + \frac{\Delta(\Delta-1)^2}{8}, & \text{for } k = 2; \\ \frac{\Delta(\Delta-1)^{k-1}}{4} \left[(\Delta-1) \left\{ 1 + \frac{1}{2} + \dots + \frac{1}{k-1} + \frac{(\Delta-1)^{k-1}}{k} \right\} - 1 \right], & \text{for } k \geq 3. \end{cases} \quad \square \end{aligned}$$

4 Computation of peripheral Harary index using adjacency matrix

Let G be a graph of diameter d with n vertices v_1, \dots, v_n . Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of G , where

$$a_{ij}^{(1)} = \begin{cases} 1, & \text{if } v_i \sim v_j; \\ 0, & \text{otherwise.} \end{cases}$$

Consider the powers A^t , $2 \leq t \leq d$ of A . We denote the (i, j) -th element of A^t ($2 \leq t \leq d$), by $a_{ij}^{(t)}$, where

$$a_{ij}^{(t)} = \sum_{k=1}^n a_{ik}^{(t-1)} a_{kj}^{(1)}.$$

We know that $a_{ij}^{(t)}$ is the number of distinct edge sequences of length t between v_i and v_j . For $i \neq j$, let $a_{ij}^{(q_{ij})}$ be the first non-zero entry in the sequence $a_{ij}^{(1)}, a_{ij}^{(2)}, \dots, a_{ij}^{(d)}$. Then, it is clear that $a_{ij}^{(q_{ij})}$ is the the number of geodesics of length q_{ij} between v_i and v_j . Therefore $d(v_i, v_j) = q_{ij}$. Note that the matrix (q_{ij}) is the distance matrix of G , where q_{ii} is set to zero.

Suppose that G has k peripheral vertices. Without loss of generality we may assume that v_1, \dots, v_k are the peripheral vertices of G (this is nothing but relabeling of vertices). Therefore from (2.1), the peripheral Harary index of G is given by

$$PH(G) = \sum_{1 \leq i < j \leq k} \frac{1}{q_{ij}} \tag{4.1}$$

Let us define $\phi_{ij}^{(t)}$, ($1 \leq t \leq d, i \neq j$) as follows:

$$\phi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \dots = a_{ij}^{(t-1)} = 0 \text{ and } a_{ij}^{(t)} \neq 0; \\ 0, & \text{otherwise.} \end{cases} \tag{4.2}$$

Then

$$q_{ij} = 1 \cdot \phi_{ij}^{(1)} + 2 \cdot \phi_{ij}^{(2)} + \dots + d \cdot \phi_{ij}^{(d)} = \sum_{t=1}^d t \cdot \phi_{ij}^{(t)} \tag{4.3}$$

Using (4.3) in (4.1), we write

$$PH(G) = \sum_{1 \leq i < j \leq k} \frac{1}{\sum_{t=1}^d t \cdot \phi_{ij}^{(t)}} \tag{4.4}$$

Thus, we have the following theorem:

Theorem 4.1. *Let G be a graph of diameter d with n vertices v_1, \dots, v_n and k peripheral vertices v_1, \dots, v_k . Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of G . Denote the (i, j) -th element of A^t ($2 \leq t \leq d$) by $a_{ij}^{(t)}$. Then*

$$PH(G) = \sum_{1 \leq i < j \leq k} \frac{1}{\sum_{t=1}^d t \cdot \phi_{ij}^{(t)}},$$

where $\phi_{ij}^{(t)}$, ($1 \leq t \leq d, i \neq j$) is given by

$$\phi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \dots = a_{ij}^{(t-1)} = 0 \text{ and } a_{ij}^{(t)} \neq 0; \\ 0, & \text{otherwise.} \end{cases}$$

4.1 An algorithm

Here, we present an algorithm to find the peripheral Harary index of a graph G using its adjacency matrix A . An algorithm for finding the distance matrix D of G is assumed.

Algorithm to find the peripheral Harary index

Input: Adjacency matrix of a connected graph G

Output: 1. $PH(G)$, peripheral Harary index of the graph G
2. P , Vector of peripheral vertices

Start:

Step 1: Define the adjacency matrix A of G

Step 2: Determine the distance matrix D of G

Step 3: Determine P

Step 3.1: [Initialize k to 1]

Step 3.2: [Determine the diameter t of the graph]

$t = D[1, 1]$

Repeat for $i = 1$ to n

Repeat for $j = 1$ to n

If $i < j$ then

if $(D[i, j] > t)$ then

$t = D[i, j]$

Step 3.3: Repeat for $j = 1$ to n

If $(D[k, j] = t)$ then

$P[k] = j$

$k = k + 1$

Step 4: Compute the Peripheral Harary index

Step 4.1: [Initialize $PH(G)$ to 0]

Step 4.2: Repeat for $i = 1$ to k

Repeat for $j = i + 1$ to k

$$PH(G) = PH(G) + 1/D[P[i], P[j]]$$

Step 5: End of the algorithm

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