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GENERALIZED HARARY INDEX OF CERTAIN CLASSES OF GRAPHS

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Abstract

A new generalized variant of the much acclaimed distance based topological index was introduced by Xu et al. and named as the generalized Harary index defined as

$$H_k(G) = \sum_{u, v \in V(G)} \frac{1}{d_G(u) + k},$$

where the summation goes over all unordered pairs of vertices in a simple and undirected graph $G = (V, E)$ and k is a fixed arbitrary non-negative real number [28]. In this article, we computed the generalized Harary indices of some special classes of graphs such as Mycielski's graphs, zero-divisor graphs and some specific families of tree-like linear alkanes, Gutman, bistar, banana and Kragujevac trees.

1. Significance of the Work

Graph theory is getting more and more popular each day due to its numerous applications and techniques in many areas including some industrial applications. Therefore, graph theory is getting more importance and is being dealt with by new methods. Topological indices are one of these methods of studying graphs and obtaining new applications of them. Since Harary applied this idea to obtain the boiling points of some alkanes in 1947, many papers have been written on mathematical properties of these indices and their applications in different fields. This work aims to be one of these papers written on mathematical properties of generalized version of the Harary index.

2. Introduction

Throughout this paper, we consider finite, connected, undirected graphs without loops and multiple edges. Such graphs will briefly be called *simple graphs*. Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The distance between the two vertices u and v denoted by $d_G(u, v)$ or $d(u, v)$ is the length of a shortest path between the vertices u and v in G.

For graph theoretical terminology and notation not defined here, we follow [10, 12].

Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that can be used to characterize some property of the graph of a molecule is called a *molecular descriptor* for that graph. There are numerous molecular descriptors, which are also referred to as topological indices that have found some applications in theoretical chemistry, especially in QSPR/QSAR/QSTR research. For their history, applications and mathematical properties, see [11, 22, 23] and the references cited therein.

The Wiener index is one of the most studied topological indices both from a theoretical point of view and applications, see [6]. It was introduced by Harold Wiener in 1947 in connection with the study of boiling points of alkane molecules based on the formula

$$\text{Boiling point} = \alpha W(G) + \beta w(3) + \gamma,$$

where α, β and γ are empirical constants and $w(3)$ is the so-called path number, namely, the number of pairs of vertices whose distance is equal to three. For more details, refer to [25]. Formally, the Wiener index of a graph G is defined as follows:

$$W(G) = \sum_{\{u, v\} \subseteq V(G)} d_G(u, v).$$

The Harary index of a graph G has been introduced independently by Plavsic et al. [20] and Ivanciuc et al. [14] in 1993. It has been named in honor of brand ambassador of graph theory Professor Frank Harary on the occasion of his 70th birthday. The Harary index of a simple connected graph G is defined as

$$H(G) = \sum_{\{u, v\} \subseteq V(G)} \frac{1}{d_G(u, v)}; \quad (u \neq v),$$

where the summation goes over all unordered pairs of vertices of G.

The above Harary index was generalized and studied by Xu et al. [28] and the generalization was defined as follows:

$$H_k(G) = \sum_{\{u, v\} \subseteq V(G)} \frac{1}{d_G(u, v) + k}; \quad (u \neq v),$$

where the summation goes over all unordered pairs of vertices of G and k is any non-negative real number.

The reciprocal distance-based graph invariants have already been extensively studied. For their applications and mathematical properties, see [4, 7, 8, 15, 16, 26, 27, 29] and the references cited therein.

3. Some Standard Graphs

Proposition 3.1. *The generalized Harary index of a complete graph* K_n *with* $n \geq 3$ *is given by*

$$H_k(K_n) = \frac{n(n-1)}{2(1+k)}.$$

Proof. For $n \geq 3$, let $G = K_n$ be a complete graph. By the definition, we have

$$H_k(G) = \sum_{\{u_i, u_j\} \subseteq V(G)} \frac{1}{d_G(u_i, u_j) + k}; \quad (u_i \neq u_j).$$

Since any two vertices in K_n are adjacent, distance between every pair of vertices is one. Therefore,

$$H_k(K_n) = \sum_{\{u_i, u_j\} \subseteq V(G)} \frac{1}{d_G(u_i, u_j) + k} = \frac{n(n-1)}{2} \frac{1}{1+k}. \qquad \square$$

Corollary 3.1. *For* $k = 0$, *the Harary index of a complete graph* K_n *for* $n \geq 3$ *is given by*

$$H(K_n) = \frac{n(n-1)}{2}.$$

Proposition 3.2. *The generalized Harary index of a cycle graph* C_n *with* $n \geq 3$ *vertices is given by*

$$H_k(G) = \begin{cases} n\sum_{r=1}^{\frac{n-1}{2}} \frac{1}{r+k}, & \text{if } n \text{ is odd}, \\ n\sum_{r=1}^{\frac{n-2}{2}} \frac{1}{r+k} + \frac{n}{n+2k}, & \text{if } n \text{ is even.} \end{cases}$$

Proof. For $n \geq 3$, let $G = C_n$ be a cycle graph. By the definition, we have

$$H_k(G) = \sum_{\{u_i, u_j\} \subseteq V(G)} \frac{1}{d_G(u_i, u_j) + k}; \quad (u_i \neq u_j).$$

Case 1. Let G be an odd cycle. Clearly starting with any vertex u_i in an odd cycle, the remaining vertices can be grouped into pairs such that both vertices in each pair are at the same distance from u_i. There are $\frac{n-1}{2}$ such pairs. Therefore,

$$\begin{aligned} H_k(G) &= \sum_{\{u_i, u_j\} \subseteq V(G)} \frac{1}{d_G(u_i, u_j) + k}; (u_i \neq u_j) \\ &= \frac{1}{2}\left[2 \sum_{j=1}^{(n-1)/2} \frac{1}{d_G(u_i, u_j) + k} \right], \text{ where } 1 \leq i \leq n \\ &= n \sum_{r=1}^{(n-1)/2} \frac{1}{r+k}. \end{aligned}$$

Case 2. Let G be an even cycle. Clearly starting with any vertex u_i in an even cycle except the vertex which is farthest from u_i, the remaining vertices can be grouped into pairs such that both vertices in each pair are at same distance from u_i. There are $\frac{n-2}{2}$ such pairs. The vertex w which is

farthest from u_i is at distance $\frac{n}{2}$ from u_i. Therefore,

$$H_k(G) = \sum_{\{u_i, u_j\} \subseteq V(G)} \frac{1}{d_G(u_i, u_j) + k}, (u_i \neq u_j)$$

$$= \frac{1}{2}\left[2 \sum_{j=1}^{\frac{n-2}{2}} \frac{1}{d_G(u_i, u_j) + k} \right] + \frac{1}{2} \frac{1}{d_G(u_i, w) + k}, \text{ where } 1 \leq i \leq n$$

$$= n\left[\sum_{r=1}^{\frac{n-2}{2}} \frac{1}{r + k} \right] + \frac{1}{2}\left[\frac{n}{\frac{n}{2} + k} \right]$$

$$= n \sum_{r=1}^{\frac{n-2}{2}} \frac{1}{r + k} + \frac{n}{n + 2k}. \qquad \square$$

Corollary 3.2. *For $k = 0$, the Harary index of a cycle C_n with $n \geq 3$ vertices is given by*

$$H(G) = \begin{cases} n \sum_{r=1}^{\frac{n-1}{2}} \frac{1}{r}, & \text{if } n \text{ is odd}, \\ n \sum_{r=1}^{\frac{n-2}{2}} \frac{1}{r} + 1, & \text{if } n \text{ is even.} \end{cases}$$

Proposition 3.3. *The generalized Harary index of a complete bipartite graph $K_{r,s}$ with $1 \leq r \leq s$ is given by*

$$H_k(K_{r,s}) = \frac{r^2 - r + s^2 - s}{2(2 + k)} + \frac{rs}{1 + k}.$$

Proof. Let $G = K_{r,s}, 1 \leq r \leq s$ be a complete bipartite graph. By the definition, we have

$$H_k(K_{r,s}) = \sum_{\{u_i, u_j\} \subseteq V(K_{r,s})} \frac{1}{d_G(u_i, u_j) + k}; \quad (u_i \neq u_j).$$

We know that $V(K_{r,s}) = V_1 \bigcup V_2$ with $|V_1| = r$, $|V_2| = s$. Then the following three cases arise:

- If $\{u_i, u_j\} \subseteq V_1$, then $d_{K_{r,s}}(u_i, u_j) = 2$. Here we have

$$\sum_{\{u_i, u_j\} \subseteq V_1} \frac{1}{d_{K_{r,s}}(u_i, u_j) + k} = \sum_{\{u_i, u_j\} \subseteq V_1} \frac{1}{2 + k} = \frac{r(r-1)}{2(2+k)}.$$

- If $\{u_i, u_j\} \subseteq V_2$, then $d_{K_{r,s}}(u_i, u_j) = 2$. Hence

$$\sum_{\{u_i, u_j\} \subseteq V_2} \frac{1}{d_{K_{r,s}}(u_i, u_j) + k} = \sum_{\{u_i, u_j\} \subseteq V_2} \frac{1}{2 + k} = \frac{s(s-1)}{2(2+k)}.$$

- If $u_i \subseteq V_1, u_j \subseteq V_2$, then $d_{K_{r,s}}(u_i, u_j) = 1$. Hence we have

$$\sum_{u_i \subseteq V_1, u_j \subseteq V_2} \frac{1}{d_{K_{r,s}}(u_i, u_j) + k} = \sum_{u_i \subseteq V_1, u_j \subseteq V_2} \frac{1}{1 + k} = \frac{rs}{1+k}.$$

From these three cases, the result follows. □

Corollary 3.3. *For $k = 0$, the Harary index of a complete bipartite graph $K_{r,s}$ with $1 \leq r \leq s$ is given by*

$$H(K_{r,s}) = \frac{r^2 - r + s^2 - s}{4} + rs.$$

Corollary 3.4. *The generalized Harary index of a regular complete bipartite graph $K_{r,r}$ with $r \geq 2$ is given by*

$$H_k(K_{r,r}) = \frac{r^2 - r}{2 + k} + \frac{r^2}{1 + k}.$$

Corollary 3.5. *For* $k = 0$, *the Harary index of a regular complete bipartite graph* $K_{r,r}$ *with* $r \geq 2$ *is given by*

$$H(K_{r,r}) = \frac{r^2 - r}{2} + r^2.$$

Theorem 3.1. *The generalized Harary index of a star graph* S_n *with* $n-1$ *pendant vertices is given by*

$$H_k(S_n) = \frac{n-1}{2}\left[\frac{n-2}{2+k} + \frac{2}{1+k}\right].$$

Proof. Let $G = S_n$ be a star graph. By the definition, we have

$$H_k(G) = \sum_{\{u_i, u_j\} \subseteq V(G)} \frac{1}{d_G(u_i, u_j) + k}; \quad (u_i \neq u_j).$$

In S_n, there are $n-1$ pendant vertices u_i with $(1 \leq i \leq n-1)$ and one vertex, say w, of degree $n-1$. There are $n-2$ pairs (u_i, u_j), where $i \neq j$ for a fixed i. So, in total, there are $(n-1)(n-2)$ pairs (u_i, u_j), where $i \neq j$ for all i, j. Moreover, $d_G(u_i, u_j) = 2$ and $d_G(w, u_j) = 1$. Therefore,

$$\begin{aligned} H_k(G) &= \frac{1}{2} \sum_{u_j \subseteq V(G),\, d_G(u_j)=1} \frac{1}{d_G(u_i, u_j) + k} \\ &\quad + \sum_{u_j \subseteq V(G),\, d_G(u_j)=1} \frac{1}{d_G(w, u_j) + k} \\ &= \frac{1}{2}\frac{(n-1)(n-2)}{2+k} + \frac{n-1}{1+k} \\ &= \left(\frac{n-1}{2}\right)\left[\frac{n-2}{2+k} + \frac{2}{1+k}\right]. \end{aligned}$$

□

Corollary 3.6. *For* $k = 0$, *the Harary index of a star graph* S_n *is given by*

$$H(S_n) = \frac{(n-1)(n+2)}{4}.$$

4. Mycielskian Graphs

Mycielski's construction is a well-known construction on graphs which produces a $(k+1)$-chromatic triangle-free graph from a k-chromatic triangle-free graph. We recall the Mycielski's construction as follows:

From a simple graph G, Mycielski's construction produces a simple graph $\mu(G)$ containing G as follows: Start with a graph G having vertex set $\{v_1, v_2, ..., v_n\}$. Add vertices $U = \{u_1, u_2, ..., u_n\}$ and one more vertex w. Add edges to make u_i adjacent to all vertices in $N_G(v_i)$ and finally let $N(w) = U$. For more details, we refer to [24] and [19].

Here, we calculate the generalized Harary index of the Mycielskian of a graph of diameter 2. To do this, we make use of the following well-known observation and lemma:

Observation 4.1 [17]**.** Let $G = (V, E)$ be a graph with n vertices and m edges. Then the number of paths of length two is equal to $\frac{1}{2}M_1(G) - m$.

Lemma 4.1 [2]**.** *Let G be a connected graph. Then the distances between the vertices of the Mycielskian graph $\mu(G)$ of G are given as follows. For each x, y in $V(\mu(G))$,*

$$\text{(i) } d_{\mu(G)}(x, y) = \begin{cases} 2, & \text{if } x = u_i,\ y = u_j, \\ d_G(v_i, v_j), & \text{if } x = v_i,\ y = v_j,\ d_G(v_i, v_j) \le 3, \\ 4, & \text{if } x = v_i,\ y = v_j,\ d_G(v_i, v_j) \ge 4, \end{cases}$$

$$\text{(ii) } d_{\mu(G)}(x, y) = \begin{cases} 2, & \text{if } x = v_i,\ y = u_j,\ i = j, \\ d_G(v_i, v_j), & \text{if } x = v_i,\ y = u_j,\ d_G(v_i, v_j) \le 2,\ i \ne j, \\ 3, & \text{if } d_G(v_i, v_j) \ge 3,\ i \ne j, \end{cases}$$

(iii) $d_{\mu(G)}(x,\ y) = \begin{cases} 2, & \text{if } x = v_i,\ y = w, \\ 1, & \text{if } x = u_i,\ y = w. \end{cases}$

Note that the diameter of a Mycielskian graph is at most 4.

Theorem 4.1. *Let G be an n-vertex graph of size m whose diameter is 2. If $\mu(G)$ is the Mycielskian of G, then the generalized Harary index of $\mu(G)$ is given by*

$$H_k(\mu(G)) = H_k(G) + \frac{2m+n}{1+k} + \frac{n^2+3n+2M_1(G)-4m}{2(2+k)}.$$

Proof. We have the definition of generalized Harary index as

$$H_k(G) = \sum_{\{u,\ v\}\subseteq V(G)} \frac{1}{d_G(u,\ v)+k}; \quad (u \neq v).$$

By the above observation and lemma, the following cases arise:

• If $\{x,\ y\} \subseteq U$, then $d_{\mu(G)}(x,\ y) = 2$. Hence

$$H_k(\mu(G)) = \sum_{\{x,\ y\}\subseteq U} \frac{1}{d_{\mu(G)}(x,\ y)+k} = \sum_{\{x,\ y\}\subseteq U} \frac{1}{2+k} = \frac{n(n-1)}{2(2+k)}.$$

• If $\{x,\ y\} \subseteq V(G)$, then $d_{\mu(G)}(x,\ y) = d_G(x,\ y)$ for each $x,\ y \in V(G)$ implying that

$$H_k(\mu(G)) = \sum_{\{x,\ y\}\subseteq V(G)} \frac{1}{d_{\mu(G)}(x,\ y)+k}$$

$$= \sum_{\{x,\ y\}\subseteq V(G)} \frac{1}{d_G(x,\ y)+k} = H_k(G).$$

• If $x = v_i,\ y = u_j, 1 \leq i \leq n$ and $i = j$, then $d_{\mu(G)}(x,\ y) = 2$. Hence

$$H_k(\mu(G)) = \sum_{\{x,\ y\}\subseteq V(\mu(G))} \frac{1}{d_{\mu(G)}(x,\ y)+k} = \sum_{\{x,\ y\}\subseteq V(\mu(G))} \frac{1}{2+k} = \frac{n}{2+k}.$$

• If $x = v_i$, $y = u_j$ and $i \neq j$, then $d_{\mu(G)}(x, y) = d_G(x, y)$. In this case, we have

$$H_k(\mu(G)) = \sum_{\{x, y\} \subseteq V(\mu(G))} \frac{1}{d_{\mu(G)}(x, y) + k}$$

$$= \sum_{xy \in E(G)} \frac{1}{1 + k} + \sum_{xy \notin E(G)} \frac{1}{2 + k}$$

$$= \frac{2m}{1 + k} + \frac{M_1(G) - 2m}{2 + k}.$$

• If $x = w$, $y = u_i$, then $d_{\mu(G)}(x, y) = 1$. Here

$$H_k(\mu(G)) = \sum_{\{x, y\} \subseteq V(\mu(G))} \frac{1}{d_{\mu(G)}(x, y) + k} = \frac{n}{1 + k}.$$

• If $x = w$, $y \in V(G)$, then $d_{\mu(G)}(x, y) = 2$. Then we have

$$H_k(\mu(G)) = \sum_{\{x, y\} \subseteq V(\mu(G))} \frac{1}{d_{\mu(G)}(x, y) + k} = \frac{n}{2 + k}.$$

From these six cases, the result follows. □

Corollary 4.1. *For $k = 0$, the Harary index of the Mycielskian of G is given by*

$$H(\mu(G)) = H(G) + \left(m + \frac{7}{4}n\right) + \frac{1}{4}[n^2 + 2M_1(G)].$$

We next find the generalized Harary index of the complement of the Mycielskian of a graph of diameter 2. To achieve this, we use the following well-known lemma:

Lemma 4.2 [2]**.** *Let $\overline{\mu}(G)$ be the complement of the Mycielskian $\mu(G)$. Then the distances between the vertices $u, v \in V(\overline{\mu}(G))$ of G are given as follows.*

$$d_{\overline{\mu}(G)}(x,\ y) = \begin{cases} 2, & if\ \ x = w,\ y = u_i, \\ 1, & if\ \ x = w,\ y = v_i, \\ 1, & if\ \ x = u_i,\ y = u_j, \\ 1, & if\ \ x = v_i,\ y = v_j,\ d_G(v_i,\ v_j) > 1, \\ 2, & if\ \ x = v_i,\ y = v_j,\ d_G(v_i,\ v_j) = 1, \\ 1, & if\ \ x = v_i,\ y = u_j,\ i = j, \\ 1, & if\ \ x = v_i,\ y = u_j,\ i \neq j,\ d_G(v_i,\ v_j) > 1, \\ 2, & if\ \ x = v_i,\ y = u_j,\ i \neq j,\ d_G(v_i,\ v_j) = 1. \end{cases}$$

Theorem 4.2. *Let G be an n-vertex graph of size m whose diameter is 2. If $\overline{\mu}(G)$ is the complement of the Mycielskian $\mu(G)$ of G, then the generalized Harary index of $\overline{\mu}(G)$ is given by*

$$H_k(\overline{\mu}(G)) = \frac{2n^2 - 3m}{1+k} + \frac{3m+n}{2+k}.$$

Proof. By the definition of generalized Harary index, we can write

$$H_k(\overline{\mu}(G)) = \sum_{\{u,\,v\}\subseteq V(\overline{\mu}(G))} \frac{1}{d_{\overline{\mu}(G)}(u,\ v) + k}; \quad (u \neq v).$$

By the above lemma, the following cases arise based on the distances between the vertices $u,\ v \in V(\overline{\mu}(G))$ of a graph G:

- If $\{x,\ y\} \subseteq U$, then $d_{\overline{\mu}(G)}(x,\ y) = 1$. Hence

$$H_k(\overline{\mu}(G)) = \sum_{\{x,\,y\}\subseteq U} \frac{1}{d_{\mu(G)}(x,\ y) + k} = \sum_{\{x,\,y\}\subseteq U} \frac{1}{1+k} = \frac{n(n-1)}{2(1+k)}.$$

- If $\{x,\ y\} \subseteq V(G)$, then $d_{\overline{\mu}(G)}(x,\ y) = 1$, for each $xy \notin E(G)$ and $d_{\overline{\mu}(G)}(x,\ y) = 2$, otherwise.

Moreover,

$$\begin{aligned} X &= \{\{x,\ y\} \subseteq V(G) : x \neq y,\ xy \notin E(G)\} \\ &= \{\{x,\ y\} \subseteq V(G) : x \neq y\} - \{\{x,\ y\} \subseteq V(G) : xy \in E(G)\}. \end{aligned}$$

Clearly, $|X| = \frac{n(n-1)}{2} - m$. Then

$$H_k(\overline{\mu}(G)) = \sum_{\{x, y\}\subseteq V(G)} \frac{1}{d_{\overline{\mu}(G)}(x, y) + k} = \sum_{xy\notin E(G)} \frac{1}{d_{\overline{\mu}(G)}(x, y) + k}$$

$$+ \sum_{xy\in E(G)} \frac{1}{d_{\overline{\mu}(G)}(x, y) + k}$$

$$= \sum_{xy\notin E(G)} \frac{1}{1+k} + \sum_{xy\in E(G)} \frac{1}{2+k}$$

$$= \left(\frac{n(n-1)}{2} - m\right)\left(\frac{1}{1+k}\right) + \frac{m}{2+k}.$$

• If $x = v_i$ and $y = u_i$, $1 \le i \le n$, $\{x, y\} \subseteq V(\overline{\mu}(G))$, then $d_{\overline{\mu}(G)}(x, y) = 1$. Here

$$H_k(\overline{\mu}(G)) = \sum_{x, y\subseteq V(\overline{\mu}(G))} \frac{1}{d_{\overline{\mu}(G)}(x, y) + k} = \sum_{i=1}^{n} \frac{1}{1+k} = \frac{n}{1+k}.$$

• If $x = v_i$ and $y = u_j$, $i \neq j$, then

$$X = \{\{x, y\} \subseteq V(G),\ x \neq y : xy \notin E(G)\}$$

$$= \{\{x, y\} \subseteq V(G),\ x \neq y\} = \{\{x, y\} \subseteq V(G) : xy \notin E(G)\}.$$

Clearly,

$$|X| = \frac{n(n-1)}{2} - m.$$

Note that

$$\sum_{(v_i, v_j),\, v_iv_j\notin E(G)} \frac{1}{d_{\overline{\mu}(G)}(v_i, v_j) + k} = 2 \sum_{\{v_i, v_j\},\, v_iv_j\notin E(G)} \frac{1}{d_{\overline{\mu}(G)}(v_i, v_j) + k}.$$

Thus,

$$\sum_{\{x,\,y\}\subseteq V(\overline{\mu}(G)),\,i\neq j}\frac{1}{d_{\mu(G)}(x,\,y)+k}=\sum_{(v_i,\,v_j),\,v_iv_j\notin E(G)}\frac{1}{d_{\overline{\mu}(G)}(v_i,\,v_j)+k}$$

$$+\sum_{v_iv_j\in E(G)}\frac{1}{d_{\overline{\mu}(G)}(v_i,\,v_j)+k}$$

$$=\frac{2\left(\frac{n(n-1)}{2}-m\right)}{1+k}+\frac{2m}{2+k}.$$

- If $x=w,\ y\in U,$ then $d_{\overline{\mu}(G)}(x,\,y)=2.$ Hence

$$\sum_{\{x,\,y\}\subseteq V(\overline{\mu}(G))}\frac{1}{d_{\overline{\mu}(G)}(x,\,y)+k}=\frac{n}{2+k}.$$

- If $x=w,\ y\in V(G),$ then $d_{\overline{\mu}(G)}(x,\,y)=1.$ In this case, we have

$$\sum_{\{x,\,y\}\subseteq V(\overline{\mu}(G))}\frac{1}{d_{\overline{\mu}(G)}(x,\,y)+k}=\frac{n}{1+k}.$$

From the above six cases, the result follows. □

Corollary 4.2. *For* $k=0,$ *we have*

$$H(\overline{\mu}(G))=\frac{1}{2}[4n^2-3m+n].$$

5. Zero Divisor Graphs

The zero divisor graph of a commutative ring R, denoted by $\Gamma[R],$ is a graph whose vertices are all non-zero zero divisors of R and two vertices are adjacent if their product is zero. Here, we consider the zero divisor graph $\Gamma[Z_n]$ or $n=p^3$ and $n=p^2q,$ where p and q are distinct primes. This concept was first initiated by Beck [5] and studied by Anderson and

Livingston [3], Akbari and Mohammadian [1], Ahmadi and Jahani-Nezhad [18] and Reddy et al. [21].

Observation 5.1. Let p be a prime number. Then

$$Z^*(Z_{p^2}) = \{p, 2p, ..., (p-1)p\} = V[\Gamma(Z_{p^2})]$$

and $d(x, y) = 1$ for all $x, y \in \Gamma(Z_{p^2})$. Clearly, $\Gamma(Z_{p^2}) = K_{p-1}$, the complete graph on $p-1$ vertices.

Theorem 5.1. *Generalized Harary index of* $\Gamma(Z_{p^2})$ *is given by*

$$H_k(\Gamma(Z_{p^2})) = \frac{(p-1)(p-2)}{2(1+k)}.$$

Proof. Clearly, we have

$$H_k(\Gamma(Z_{p^2})) = \sum_{u \neq v,\, u, v \in V(\Gamma(Z_{p^2}))} \frac{1}{d_G(u, v) + k}$$

$$= \frac{(p-1)(p-2)}{2}\left(\frac{1}{1+k}\right). \qquad \square$$

Observation 5.2. If p and q are prime numbers, then $\Gamma(Z_{pq}) \cong K_{p-1, q-1}$ with $Z^*|(Z_{pq}) = A \cup B = V(\Gamma(Z_{pq}))$, where

$$A = \{k_1 p : k_1 = 1, 2, ..., q-1\}$$

and

$$B = \{k_2 q : k_2 = 1, 2, ..., p-1\}.$$

Let $A_1 = \{\text{If } x \in A, y \in B, d(x, y) = 1\}$. Then $|A_1| = p-1$. The number of such pairs is $p-1$. Let $A_2 = \{\text{If } x \in A, y \in A, x \neq y, d(x, y) = 2\}$, where $|A_2| = q-2$. The number of such pairs is $p-2$. Clearly, $|A_1| + |A_2| = q-1$. Let $A_3 = \{\text{If } x \in B, y \in A, d(x, y) = 1\}$, where $|A_3|$

$= q-1$. Let $A_4 = \{\text{If } x \in B,\ y \in B,\ d(x,\ y) = 2\}$, where $|A_1| = p-2$. Clearly, $|A_3| + |A_4| = p-1$.

Theorem 5.2. *The generalized Harary index of* $\Gamma(Z_{pq})$ *is given by*

$$H_k(\Gamma(Z_{pq})) = \frac{(p-1)(q-1)}{1+k} + \frac{p+q-4}{2(2+k)}.$$

Proof. Consider

$$H_k(\Gamma(Z_{pq})) = \sum_{u \neq v,\ u,\ v \in V(\Gamma(Z_{p^2}))} \frac{1}{d_G(u,\ v)+k}$$

$$= \frac{1}{2}\left[(q-1)\left\{\frac{p-1}{1+k} + \frac{q-2}{2+k}\right\}\right]$$

$$+ \frac{1}{2}\left[(p-1)\left\{\frac{q-1}{1+k} + \frac{p-2}{2+k}\right\}\right].$$

Thus the result follows. □

Observation 5.3. Let $\Gamma(Z_{p^3})$ be a zero divisor graph with $V(\Gamma(Z_{p^3})) = A \cup B = V$, where $A = \{k_1 p : k_1 = 1,\ 2,\ ...,\ p^2 - 1;\ k_1 \mid p\}$; $|A| = p^2 - p - r$, and $B = \{k_2 p^2 : k_2 = 1,\ 2,\ ...,\ p-1\}$; $|B| = p - 1 = s$. Then the following cases arise:

$$A_1 = \{\text{If } x \in A,\ y \in A,\ d(x,\ y) = 2\}; \quad |A_1| = \frac{r(r-1)}{2},$$

$$A_2 = \{\text{If } x \in B,\ y \in B,\ d(x,\ y) = 1\}; \quad |A_2| = \frac{s(s-1)}{2},$$

$$A_3 = \{\text{If } x \in A,\ y \in B,\ d(x,\ y) = 1\}; \quad |A_3| = rs.$$

Theorem 5.3. *The generalized Harary index of the zero divisor graph* $\Gamma(Z_{p^3})$ *is given by*

$$H_k(\Gamma(Z_{p^3})) = \frac{p-1}{2}\left(\frac{p(p^2-p-1)}{2+k} + \frac{2p^2-p-1}{1+k}\right).$$

Proof. Let $\Gamma(Z_{p^3})$ be the zero divisor graph of Z_{p^3}. Then we have

$$\begin{aligned}
H_k(\Gamma(Z_{p^3})) &= \sum_{u\neq v,\ u,v\in V(\Gamma(Z_{p^3}))} \frac{1}{d_G(u,v)+k} \\
&= \sum_{u,v\in A} \frac{1}{d_G(u,v)+k} + \sum_{u,v\in B} \frac{1}{d_G(u,v)+k} \\
&\quad + \sum_{u\in A,\ v\in B} \frac{1}{d_G(u,v)+k} \\
&= \frac{r(r-1)}{2(2+k)} + \frac{s(s-1)}{2(1+k)} + \frac{rs}{1+k} \\
&= \frac{(p^2-p)(p^2-p-1)}{2(2+k)} + \frac{(p-1)(p-2)}{2(1+k)} + \frac{p(p-1)^2}{1+k} \\
&= \frac{p-1}{2}\left[\frac{p^3-p^2-p}{2+k} + \frac{p-2}{1+k} + \frac{2(p^2-p)}{1+k}\right] \\
&= \frac{p-1}{2}\left(\frac{p(p^2-p-1)}{2+k} + \frac{2p^2-p-1}{1+k}\right).
\end{aligned}$$

□

Observation 5.4. Let $\Gamma(Z_{p^2q})$, where p and q are distinct prime numbers with $V(\Gamma(Z_{p^2q})) = A \cup B \cup C \cup D$, where

$$A = \{k_1 p : k_1 = 1, 2, ..., pq-1, k_1 \mid pq\}; \quad |A| = (p-1)(q-1) = a,$$

$$B = \{k_2 q : k_2 = 1, 2, ..., p^2-1, k_2 \mid p\}; \quad |B| = p(p-1) = b,$$

$$C = \{k_3 pq : k_3 = 1, 2, ..., p-1\}; \quad |C| = q-1 = c,$$

$$D = \{k_4 p^2 : k_4 = 1, 2, ..., q^2-1\}; \quad |D| = p-1 = d.$$

Then the following cases arise:

$$A_1 = \{\text{If } x, y \in A, d(x, y) = 2\}; \quad |A_1| = \frac{a(a-1)}{2},$$

$$A_2 = \{\text{If } x, y \in B, d(x, y) = 2\}; \quad |A_2| = \frac{b(b-1)}{2},$$

$$A_3 = \{\text{If } x, y \in C, d(x, y) = 2\}; \quad |A_3| = \frac{c(c-1)}{2},$$

$$A_4 = \{\text{If } x, y \in D, d(x, y) = 1\}; \quad |A_4| = \frac{d(d-1)}{2},$$

$$A_5 = \{\text{If } x \in A, y \in B, d(x, y) = 2\}; \quad |A_5| = ab,$$

$$A_6 = \{\text{If } x \in A, y \in C, d(x, y) = 2\}; \quad |A_6| = ac,$$

$$A_7 = \{\text{If } x \in A, y \in D, d(x, y) = 1\}; \quad |A_7| = ad,$$

$$A_8 = \{\text{If } x \in B, y \in C, d(x, y) = 1\}; \quad |A_8| = bc,$$

$$A_9 = \{\text{If } x \in B, y \in D, d(x, y) = 2\}; \quad |A_9| = bd,$$

$$A_{10} = \{\text{If } x \in C, y \in D, d(x, y) = 1\}; \quad |A_{10}| = cd.$$

Theorem 5.4. *The generalized Harary index of the zero divisor graph* $\Gamma(Z_{p^2q})$ *is given by*

$$H_k(\Gamma(Z_{p^2q})) = \frac{1}{2+k}\left[\frac{a^2+b^2+c^2-(a+b+c)+2(ab+ac+bd)}{2}\right] + \frac{1}{1+c}\left[\frac{d^2-d+2(ad+bc+cd)}{2}\right].$$

Proof. Let $G = \Gamma(Z_{p^2q})$ be the zero-divisor graph of Z_{p^2q}, where p and q are distinct prime numbers. Then we have

$$H_k(\Gamma(Z_{p^2q})) = \sum_{u,v\in V(\Gamma(Z_{p^2q}))} \frac{1}{d_G(u,v)+k}$$

$$= \sum_{u,v\in A_i,1\le i\le 4} \frac{1}{d_G(u,v)+k} + \sum_{u,v\in A_j,5\le j\le 10} \frac{1}{d_G(u,v)+k}$$

$$= \frac{1}{2+k}\frac{a(a-1)}{2} + \frac{1}{2+k}\frac{b(b-1)}{2} + \frac{1}{2+k}\frac{c(c-1)}{2}$$

$$+ \frac{1}{1+k}\frac{d(d-1)}{2} + \frac{1}{2+k}ab + \frac{1}{2+k}ac$$

$$+ \frac{1}{1+k}ad + \frac{1}{1+k}bc + \frac{1}{2+k}bd + \frac{1}{1+k}cd$$

$$= \frac{1}{2(2+k)}[a(a-1)+b(b-1)+c(c-1)]$$

$$+ \frac{1}{2(1+k)}[d(d-1)] + \frac{1}{2+k}[ab+ac+bd]$$

$$+ \frac{1}{1+k}[ad+bc+cd]$$

$$= \frac{1}{2+k}\left[\frac{a^2+b^2+c^2-(a+b+c)+2(ab+ac+bd)}{2}\right]$$

$$+ \frac{1}{1+c}\left[\frac{d^2-d+2(ad+bc+cd)}{2}\right]. \qquad \square$$

6. Linear Alkanes

An alkane is an organic compound made strictly of carbons single bonded to each other or hydrogens and mostly which are derived from petroleum and petroleum byproducts. Particularly, the *n*-alkane is the least branched while the "star graph" in which all vertices are neighbors to a single central vertex is the most branched.

Theorem 6.1. *The generalized Harary index of n-alkanes G is given by*

$$H_k(G) = (n+k)\sum_{r=1}^{n-1}\frac{1}{r+k} - (n-1).$$

Proof. Let G be an n-alkane, $n \geq 2$. By the definition, we have

$$\begin{aligned}
H_k(G) &= \sum_{\{u_i,\, u_j\}\subseteq V(G)} \frac{1}{d_G(u_i,\, u_j)+k},\ (u_i \neq u_j)\\
&= \sum_{j=2}^{n}\frac{1}{d_G(u_1,\, u_j)+k} + \sum_{j=3}^{n}\frac{1}{d_G(u_2,\, u_j)+k}\\
&\quad + \cdots + \frac{1}{d_G(u_{n-1},\, u_n)+k}\\
&= \sum_{j=2}^{n}\frac{1}{(j-1)+k} + \sum_{j=3}^{n}\frac{1}{(j-1)+k} + \cdots + \frac{1}{1+k}\\
&= \frac{n-1}{1+k} + \frac{n-2}{2+k} + \cdots + \frac{n-(n-1)}{(n-1)+k}\\
&= n\sum_{r=1}^{n-1}\frac{1}{r+k} - \sum_{r=1}^{n-1}\frac{r}{r+k}\\
&= \sum_{r=1}^{n-1}\frac{n-r}{r+k} = \sum_{r=1}^{n-1}\left(\frac{n+k}{r+k} - 1\right)\\
&= (n+k)\sum_{r=1}^{n-1}\frac{1}{r+k} - (n-1).
\end{aligned}$$

□

Corollary 6.1. *For $k = 0$, the Harary index of an n-alkane G is given by*

$$H(G) = n\sum_{r=1}^{n-1}\frac{1}{r} - (n-1).$$

7. Gutman Trees

When m_i vertices of degree one are added to the ith vertex of a path graph P_p, a Gutman tree (or a caterpillar tree) denoted by $T_p(m_1, m_2, ..., m_p)$ is obtained. It is a graph consisting of a path together with some pendant vertices which have distance at most 1 to the path. Since these trees can be made to generate resonance relations among the rings (hexagons) of unbranched benzenoid hydrocarbons, the name benzenoid trees has also been suggested [9]. Clearly, $T_p(0, 0, ..., 0)$ is the path P_p. If $m_i \leq 2$ for each $2 \leq i \leq p-1$ and $m_1 \leq 3$ and $m_p \leq 3$, then it is a chemical tree.

Theorem 7.1. *Let $G = T_p(m_1, m_2, ..., m_p)$ be a Gutman tree. Then the generalized Harary index of G is*

$$\begin{aligned} H_k(G) = \frac{1}{2(2+k)}\left[\sum_{i=1}^{p} m_i(m_i - 1)\right] \\ + \sum_{i=1}^{p-1}\sum_{r=3}^{p-i+2} \frac{m_i m_{i+r-2}}{r+k} \\ + (m_1 + m_p)\sum_{r=1}^{p} \frac{1}{r+k} \\ + \sum_{s=2}^{p-1} m_s\left[\sum_{r=1}^{s-1} \frac{1}{r+1+k} + \sum_{r=1}^{p-(s-1)} \frac{1}{r+k}\right] \\ + (p+k)\sum_{r=1}^{p-1} \frac{1}{r+k} - (p-1). \end{aligned}$$

Proof. By the definition of generalized Harary index, we have

$$H_k(G) = \sum_{\{u, v\} \subseteq V(G)} \frac{1}{d_G(u, v) + k}, \ (u \neq v).$$

Let the vertex set $V(G)$ of G be divided into the subsets A_i and B as follows:

$$A_i = \{u_i : u_i \text{ is a pendant vertex at vertex } v_i \text{ of } P_p\}, \quad |A_i| = m_i,$$

$$B = \{u_i : u_i \text{ is a vertex of } P_p\}, \quad |B| = p.$$

The following cases arise:

Case 1. If $u_i, u_j \in A_i$, then $d_G(u_i, u_j) = 2$ giving

$$\sum_{\{u_i, u_j\} \subseteq A_i} \frac{1}{d_G(u_i, u_j) + k} = \frac{1}{2(2+k)} \left[\sum_{i=1}^{p} m_i(m_i - 1) \right].$$

Case 2. If $u_i \in A_i$, $u_j \in A_j$ $(i \neq j)$, then

$$\begin{aligned} \sum_{u_i \in A_i, u_j \in A_j} \frac{1}{d_G(u_i, u_j) + k} &= \left[\frac{m_1 m_2}{3+k} + \frac{m_1 m_3}{4+k} + \cdots + \frac{m_1 m_p}{p+1+k} \right] \\ &\quad + \left[\frac{m_2 m_3}{3+k} + \frac{m_2 m_4}{4+k} + \cdots + \frac{m_2 m_p}{p+k} \right] \\ &\quad + \cdots + \left[\frac{m_{p-1} m_p}{3+k} \right] \\ &= \sum_{i=1}^{p-1} \sum_{r=3}^{p-i+2} \frac{m_i m_{i+r-2}}{r+k}. \end{aligned}$$

Case 3. If $u_i \in A_i$, $u_j \in B$, then

$$\begin{aligned} \sum_{u_i \in A_i, u_j \in B} \frac{1}{d_G(u_i, u_j) + k} &= (m_1 + m_p) \sum_{r=1}^{p} \frac{1}{r+k} \\ &\quad + m_2 \left[\frac{1}{2+k} + \sum_{r=1}^{p-1} \frac{1}{r+k} \right] \end{aligned}$$

$$+ m_3\left[\sum_{r=1}^{2}\frac{1}{r+1+k}+\sum_{r=1}^{p-2}\frac{1}{r+k}\right]$$

$$+\cdots+ m_{p-1}\left[\sum_{r=1}^{p-2}\frac{1}{r+1+k}+\sum_{r=1}^{p-2}\frac{1}{r+k}\right]$$

$$= (m_1+m_p)\sum_{r=1}^{p}\frac{1}{r+k}$$

$$+\sum_{s=2}^{p-1}m_s\left[\sum_{r=1}^{s-2}\frac{1}{r+1+k}+\sum_{r=1}^{p-(s-1)}\frac{1}{r+k}\right].$$

Case 4. If $u_i, u_j \in B$, then

$$\sum_{\{u_i,\, u_j\}\subseteq B}\frac{1}{d_G(u_i,\, u_j)+k} = (p+k)\sum_{r=1}^{p-1}\frac{1}{r+k}-(p-1).$$

From these cases, the desired result follows. □

Corollary 7.1. *For $k=0$, the Harary index of a Gutman tree $T_p(m_1, m_2, ..., m_p)$ is*

$$H(T_p(m_1, m_2, ..., m_p)) = \frac{1}{4}\left[\sum_{i=1}^{p}m_i(m_i-1)\right]+\sum_{i=1}^{p-1}\sum_{r=3}^{p-i+2}\frac{m_i m_{i+r-2}}{r}$$

$$+(m_1+m_p)\sum_{r=1}^{p}\frac{1}{r}+\sum_{s=2}^{p-1}m_s\left[\sum_{r=1}^{s-1}\frac{1}{r+1}+\sum_{r=1}^{p-(s-1)}\frac{1}{r}\right]$$

$$+\ p\sum_{r=1}^{p-1}\frac{1}{r}-(p-1).$$

To prove our next result, we make use of the following definitions:

Let $T(a, b, p)$ be a tree with n vertices and diameter d obtained by linking centers of two stars with a path P_p $(p \geq 2)$. Let $a \geq 0, b \geq 0$ be the number of pendant vertices at both ends of the path P_p. Clearly, $n = a + b + p$ and $d = p + 1$. If $a = 0$ or $b = 0$, the tree $T(a, b, p)$ is called a *Broom graph* $B_{n-a, p}$ of $n - a$ vertices which has a path P_p with p vertices. If $p = 2$, $d = 3$ and $a = b$, then $T(a, b, p)$ is called a *bistar* denoted by $B_{a, a}$.

Theorem 7.2. *Let $T(a, b, p)$ be a tree with n vertices constructed as above. Then the generalized Harary index of $T(a, b, p)$ is*

$$H_k(G) = \frac{1}{2}\left[\frac{a(a-1) + b(b-1)}{2 + k}\right] + \frac{ab}{d + k} + (n + k)\sum_{r=1}^{p}\frac{1}{r + k} - p.$$

Proof. By the definition of generalized Harary index, we have

$$H_k(T(a, b, p)) = \sum_{\{u, v\} \subseteq V(T(a, b, p))} \frac{1}{d_{T(a, b, p)}(u, v) + k}; \quad (u \neq v).$$

Let the vertex set $V(T(a, b, p))$ of $T(a, b, p)$ be divided into three subsets A, B, C as follows:

$$A = \{u_i : u_i \text{ is a pendant vertex at the left end of } P_p\}, \quad |A| = a,$$

$$B = \{u_i : u_i \text{ is a pendant vertex at right end of } P_p\}, \quad |B| = b$$

and

$$C = \{u_i : u_i \text{ is a vertex of } P_p\}, \quad |C| = p.$$

The following cases arise:

Case 1. If $u_i, u_j \in A$, then

$$\sum_{\{u_i, u_j\}\subseteq A} \frac{1}{d_{T(a,b,p)}(u_i, u_j)+k} = \frac{a(a-1)}{2(2+k)}.$$

Case 2. If $u_i, u_j \in B$, then

$$\sum_{\{u_i, u_j\}\subseteq B} \frac{1}{d_{T(a,b,p)}(u_i, u_j)+k} = \frac{b(b-1)}{2(2+k)}.$$

Case 3. If $u_i \in A$, $u_j \in B$, then

$$\sum_{u_i\in A, u_j\in B} \frac{1}{d_{T(a,b,p)}(u_i, u_j)+k} = \frac{ab}{d+k}.$$

Case 4. If $u_i \in A$, $u_j \in C$, then

$$\sum_{u_i\in A, u_j\in C} \frac{1}{d_{T(a,b,p)}(u_i, u_j)+k} = a\sum_{r=1}^{p} \frac{1}{r+k}.$$

Case 5. If $u_i \in B$, $u_j \in C$, then

$$\sum_{u_i\in B, u_j\in C} \frac{1}{d_{T(a,b,p)}(u_i, u_j)+k} = b\sum_{r=1}^{p} \frac{1}{r+k}.$$

Case 6. If $u_i, u_j \in C$, then

$$\sum_{\{u_i, u_j\}\subseteq C} \frac{1}{d_{T(a,b,p)}(u_i, u_j)+k} = (p+k)\sum_{r=1}^{p-1} \frac{1}{r+k} - (p-1).$$

From these cases, the result follows. □

Corollary 7.2. *For* $k = 0$, *the Harary index of* $T(a, b, p)$ *is*

$$H(G) = \left[\frac{a(a-1)+b(b-1)}{4}\right] + \frac{ab}{d} + n\sum_{r=1}^{p}\frac{1}{r} - p.$$

Corollary 7.3. *For* $a = 0$, *the generalized Harary index of the Broom graph* $B_{n-a,\,p}$ *is*

$$H_k(B_{n-a,\,p}) = \left[\frac{b(b-1)}{2(2+k)}\right] + (b+p+k)\sum_{r=1}^{p}\frac{1}{r+k} - p.$$

Corollary 7.4. *The generalized Harary index of the bistar graph* $B_{a,a}$ *is*

$$H_k(B_{a,a}) = \left[\frac{a^2-a}{2+k}\right] + \frac{a^2}{3+k} + (2a+2+k)\sum_{r=1}^{2}\frac{1}{r+k} - 2.$$

Theorem 7.3. *Let* $T(a, b, p)$ *which is not isomorphic to* K_2 *be a tree with n vertices, m edges and diameter d constructed as above. Then*

$$H_k(T(a, b, p)) \geq \left[\frac{m}{1+k}\right] + \left[\frac{(a+b)^2 + (2p-3)(a+b) + (p-2)(p-1)}{2(d+k)}\right]$$

and

$$H_k(T(a, b, p)) \leq \left[\frac{m}{1+k}\right] + \left[\frac{(a+b)^2 + (2p-3)(a+b) + (p-2)(p-1)}{2(2+k)}\right],$$

with bounds on both the sides are attained if and only if G is isomorphic to a graph of diameter 2.

Proof. For $\{u_i, u_j\} \subseteq V(T(a, b, p))$, such that u_i and u_j are non-adjacent, we have the relation $2 \leq d_{T(a,\,p,\,b)}(u_i, u_j) \leq d$. The generalized Harary index of $T(a, b, p)$ is

$$H_k(G) = \frac{1}{2}\left[\frac{a(a-1)+b(b-1)}{2+k}\right] + \frac{ab}{d+k} + (n+k)\sum_{r=1}^{p}\frac{1}{r+k} - p$$

$$\geq \frac{1}{2}\left[\frac{a(a-1)+b(b-1)}{2+k}\right] + \frac{ab}{d+k} + (a+b)\sum_{r=1}^{p}\frac{1}{r+k}$$

$$+ (p+k)\sum_{r=1}^{p-1}\frac{1}{r+k} - (p-1)$$

$$= \left[\frac{a+b+p-1}{1+k}\right] + \left[\frac{a(a-1)+b(b-1)+2ab}{2(d+k)}\right]$$

$$+ \frac{(p-1)(a+b)}{d+k} + \sum_{r=0}^{p-2}\frac{r}{d+k}$$

$$H_k(G) \geq \left[\frac{m}{1+k}\right] + \left[\frac{(a+b)^2 + (2p-3)(a+b)}{2(d+k)}\right]$$

$$+ \left[\frac{1}{d+k}\right]\left[\frac{(p-2)(p-1)}{2}\right].$$

Hence, the result follows. If G is a graph of diameter 2, then

$$d_{T(a,b,p)}(u_i, u_j) = 2.$$

Clearly, the lower bound is attained. Similarly, we can prove that the upper bound is attained for a graph of diameter 2. □

8. Banana Trees

A graph is said to be a *banana tree* if the graph is obtained by connecting one pendant vertex of each of t-copies of an n-star graph with a single root vertex that is distinct from all the stars and it is denoted by $B_{t,n}$. For $n \leq 5$ and $t \leq 4$, $B_{t,n}$ represents a chemical tree.

Theorem 8.1. *Let $G = B_{t,n}$ be a banana tree. Then*

$$H_k(G) = \frac{nt}{1+k} + \frac{t[(n-1)(n-2)+t+1]}{2(2+k)} + \frac{t[n-3+t]}{3+k}$$

$$+ \frac{t(t-1)(2n-3)}{2(4+k)} + \frac{t(t-1)(n-2)}{5+k} + \frac{t(t-1)(n-2)^2}{2(6+k)}.$$

Proof. By the definition of generalized Harary index, we have

$$H_k(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u,v)+k}; \quad (u \neq v).$$

The following cases arise:

Case 1. If $u_i, u_j \in$ same n-star graph S_n, then

$$\sum_{\{u_i, u_j\}\subseteq S_n} \frac{1}{d_G(u_i, u_j)+k} = t\left(\frac{n-1}{2}\right)\left[\frac{n-2}{2+k} + \frac{2}{1+k}\right].$$

Case 2. If $u_i \in S_{n_i}, u_j \in S_{n_j}$ $(i \neq j)$, then

$$\sum_{u_i\in S_{n_i}, u_j\in S_{n_j}} \frac{1}{d_G(u_i, u_j)+k}$$

$$= \binom{t}{2}\left[\frac{1}{2+k} + \frac{2}{3+k} + \frac{2n-3}{4+k} + \frac{2n-4}{5+k} + \frac{(n-2)^2}{6+k}\right].$$

Case 3. If $u_i \in S_n$, u_j is the single root vertex, then

$$\sum_{u_i\in S_n, u_j} \frac{1}{d_G(u_i, u_j)+k} = t\left[\frac{1}{1+k} + \frac{1}{2+k} + \frac{n-2}{3+k}\right].$$

From these cases, the result follows. □

Corollary 8.1. *For* $k = 0$, *the Harary index of* $G = B_{t,n}$ *is*

$$H(G) = nt + \frac{t[(n-1)(n-2)+t+1]}{4} + \frac{t[n-3+t]}{3}$$

$$+ \frac{t(t-1)(10n^2+14n-53)}{120}.$$

Corollary 8.2. *For* $n \le 5$ *and* $t \le 4$, *the generalized Harary index of* $G = B_{t,n}$ *satisfies the inequality*

$$H_k(G) \le \frac{20}{1+k} + \frac{34}{2+k} + \frac{24}{3+k} + \frac{42}{4+k} + \frac{36}{5+k} + \frac{54}{6+k}.$$

Equality is attained for $B_{4,5}$.

9. Kragujevac Trees

A proper Kragujevac tree is a tree possessing a central vertex of degree at least 3, to which branches of the form A_1 and (or) A_2 and (or) A_3 and (or) … are attached. This concept was first proposed by Hosseini et al. [13].

Theorem 9.1. *Let* T_{kg} *be a Kragujevac tree with* $t \ge 2$. *Then*

$$H_k(T_{kg}) = \left[\left(\sum_{i=1}^{t} 2m_i\right) + t\right]\left(\frac{1}{1+k}\right)$$

$$+ \frac{1}{2}\left[\left(\sum_{i=1}^{t} m_i^2 + 3m_i\right) + t^2 - t\right]\left(\frac{1}{2+k}\right)$$

$$+ \left[\sum_{i=1}^{t} m_i^2 + \sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}(m_i + m_{i+r-2})\right]\left(\frac{1}{3+k}\right)$$

$$+\left\{\frac{1}{2}\sum_{i=1}^{t} m_i(m_i-1)+\sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}[(m_i+m_{i+r-2})+m_i m_{i+r-2}]\right\}$$

$$\times\left(\frac{1}{4+k}\right)+\left(\sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2} m_i m_{i+r-2}\right)\left(\frac{2}{5+k}+\frac{1}{6+k}\right).$$

Proof. By the definition of generalized Harary index, we have

$$H_k(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d_G(u,v)+k};\quad (u\neq v).$$

Let $A_i = v_i : v_i$ be a vertex in B_i and $|A_i| = m_i$. The following cases arise:

Case 1. If $u_i, u_j \in A_i$, then

$$\sum_{\{u_i,u_j\}\in A_i}\frac{1}{d_G(u_i,u_j)+k}=\sum_{i=1}^{t}\left\{2m_i\left(\frac{1}{1+k}\right)+\left[m_i+\binom{m_i}{2}\left(\frac{1}{2+k}\right)\right]\right.$$

$$\left.+2\binom{m_i}{2}\left(\frac{1}{3+k}\right)+\binom{m_i}{2}\left(\frac{1}{4+k}\right)\right\}.$$

Case 2. If $u_i \in A_i$ and $u_j \in A_j$, then

$$\sum_{u_i\in A_i,\,u_j\in A_j}\frac{1}{d_G(u_i,u_j)+k}=\frac{(t-1)}{2(2+k)}$$

$$+\sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}\left\{(m_i+m_{i+r-2})\left(\frac{1}{3+k}+\frac{1}{4+k}\right)\right.$$

$$\left.+m_i m_{i+r-2}\left(\frac{1}{4+k}+\frac{2}{5+k}+\frac{1}{6+k}\right)\right\}.$$

Case 3. If $u_i \in A_i$ and w is the central vertex, then

$$\sum_{u_i \in A_i,\, v_i = w} \frac{1}{d_G(u_i,\, w) + k} = \frac{t}{(1+k)} + \sum_{i=1}^{t} m_i \left(\frac{1}{2+k} + \frac{1}{3+k} \right).$$

From the above three cases, the result follows. □

Corollary 9.1. *For $k = 0$, the Harary index of a Kragujevac tree T_{kg} is*

$$H(T_{kg}) = \frac{t^2 + 3t}{4} + \sum_{i=1}^{t} \left(\frac{17 m_i^2 + 63 m_i}{24} \right)$$

$$+ \frac{7}{12} \sum_{i=1}^{t-1} \sum_{r=3}^{t-i+2} (m_i + m_{i+r-2})$$

$$+ \frac{49}{60} \sum_{i=1}^{t-1} \sum_{r=3}^{t-i+2} m_i m_{i+r-2}.$$

10. Results and Discussion

Topological indices are one of the most widely used methods of studying graphs and obtaining new applications. Since Wiener applied this idea to obtain the boiling points of some alkanes in 1947, many papers have been written on mathematical properties of these indices and their applications in different fields. A new generalized variant of one of the frequently studied distance based topological index introduced by Xu et al. was defined as

$$H_k(G) = \sum\nolimits_{u,\, v \in V(G)} \frac{1}{d_G(u) + k},$$

where the summation goes over all unordered pairs of vertices of a simple and undirected graph $G = (V,\, E)$ and k is a fixed arbitrary non-negative real number, [28]. In this article, we computed the generalized Harary indices of some special classes of graphs such as Mycielskian graphs, zero-divisor graphs and some specific families of tree-like linear alkanes, Gutman, bistar, banana and Kragujevac trees.

11. Conclusions

In the present paper, we calculated the generalized Harary indices of several popular graphs and graph classes which are frequently used in graph theory for several purposes, both theoretical and applied.

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