ADV MATH SCI JOURNAL
Advances in Mathematics: Scientific Journal **9** (2020), no.11, 9319–9328
ISSN: 1857-8365 (printed); 1857-8438 (electronic)
https://doi.org/10.37418/amsj.9.11.36 Spec. Iss. on ICMMSIS-2020

BOUNDS ON HARARY INDEX WITH RESPECT TO VERTEX CONNECTIVITY, INDEPENDENT NUMBER AND INDEPENDENT DOMINATION NUMBER OF A GRAPH

VINAYAK V. MANJALAPUR[1] AND MAHADEV B. ROTTI

ABSTRACT. In the present paper, we obtain bounds for Harary index $H(G)$ of a connected (molecular) graph in terms of vertex connectivity, independent number, independent domination number and characterize graphs extremal with respect to them.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G) = \{v_{1,}v_{2,}...., v_n\}$ and edge set $E(G)$. Distance between the vertices u and v in a graph G is defined as the length of shortest path between u and v, is denoted by $d(u, v)$.

Harary index $H(G)$ of a graph G is introduced independently by Plavsic et al. [4] and Ivanciuc et al. [2] in 1993 for the characterization of molecular graphs and it is defined as

$$H(G) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{1}{d(u, v)}. \tag{1.1}$$

Harary index correlate well with many chemical properties like QSPR (quantitative structure-property relationship), QSAR (quantitative structure-activity relationship) and such has been well studied over the last 25 years. Use of Harary

[1]*corresponding author*

2020 *Mathematics Subject Classification.* 05C09, 05C12.

Key words and phrases. Vertex connectivity, independence number, independence domination number, Harary index.

index in combination with other descriptors appears to be very efficacious in improving the QSPR models [6]. There is lot of mathematical and chemical literatutre's on the Harary index; for details, see the reviews and references cited therein [3–8]. For other undefined notations and terminology readers may refer [1].

The reciprocal distance number of a vertex u in a graph G is denoted by $RD(u|G)$, is defined as

$$RD(u|G) = \frac{1}{d(u|G)} = \sum_{v \in V(G)} \frac{1}{d(u,v)}. \tag{1.2}$$

From (1.2) we can rewrite (1.1) as follows

$$H(G) = \frac{1}{2} \sum_{u \in V(G)} RD(u|G). \tag{1.3}$$

The paper is classified as follows. In section 2, we have given some existing results and basic definitions. In section 3, we derive lower and upper bounds for $H(G)$ in terms of n, m, vertex connectivity (r), independent number (β_0), independent domination number (γ_0) and characterize graphs extremal with respect to them.

2. Preliminaries

Let $G = (V, E)$ be a graph and v be any vertex in G. The *degree* of a vertex in G is the number of edges incident to it and is denoted by $deg(v)$. The *eccentricity* $e(v)$ of vertex v in G is defined to be

$$e(v) = \max\{d(u,v)|u \in V\}.$$

The *radius* and the *diameter* of a graph G are denoted by $rad(G)$ and $diam(G)$, defined as

$$rad(G) = \min\{e(v)|v \in V\}$$

and

$$diam(G) = \max\{e(v)|v \in V\}.$$

Definition 2.1. *The vertex connectivity(connectivity) r of a graph G is defined as deletion of minimum number of vertices required to disconnect the graph.*

Definition 2.2. *A set $S \subseteq V(G)$ is said to be an independent set, if no two vertices of set S are adjacent. The independent number $\beta_0(G)$ is the maximum cardinality of independent sets in G.*

Definition 2.3. *In a graph G, a set $S \subseteq V(G)$ is a dominating set if every vertex not in S is adjacent to atleast one vertex of S. The domination number $\gamma(G)$ is the minimum cardinality of dominating set in G.*

Definition 2.4. *A set S is said to be independent dominating set if it is both independent and dominating set. The minimum cardinality of independent dominating set is independent domination number $\gamma_0(G)$.*

Following are the some known results which are helpful in the later proof.

Theorem 2.1. *[8] Let G be a connected graph with $n \geq 2$ vertices. Then*

$$H(P_n) + \frac{m-n+1}{2} \leq H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2}\ .$$

Theorem 2.2. *[3] For each $r = 1, 2, 3, \ldots, n-1$, the graph $K(n-1, r)$ is the unique one with the maximum Harary index among all graphs of order n and vertex connectivity r.*

Corollary 2.1. *[3] Let G be a graph of order n with vertex or edge connectivity r, where $1 \leq r \leq n-2$. Then*

$$H(G) \leq \frac{(n-1)^2 + r}{2}, \tag{2.1}$$

with equality if and only if $G = K(n-1, r)$.

3. Main Results

Following Theorem 3.1 gives upper bound for $H(G)$ in terms of n and m.

Theorem 3.1. *Let G be a graph of order n, size m with $diam(G) \geq 3$, then*

$$H(G) \leq \frac{3n(n-1) + 6m - 2}{12}. \tag{3.1}$$

Equality holds if G contains exactly two vertices of eccentricity three and rest are of eccentricity two.

Proof. Let $u \in V(G)$, be any arbitrary vertex, then we have $S_1 = \{u \in V|e(u) = 2\}$ and $S_2 = \{u \in V|e(u) \geq 3\}$. Then, $|S_1| + |S_2| = n$. If $u \in S_1$, then from the proof of Theorem 2.1, we get

$$RD(u|G) = \frac{n-1+deg(u)}{2}. \tag{3.2}$$

If $u \in S_2$, define three sets $S_{21} = \left\{v \in V|{}^1\!/_{d(u,v)} = 1\right\}$, $S_{22} = \left\{v \in V|{}^1\!/_{d(u,v)} = \frac{1}{2}\right\}$ and $S_{23} = \left\{v \in V|{}^1\!/_{d(u,v)} = \frac{1}{3}\right\}$. Clearly, $|S_{21}| + \frac{|S_{22}|}{2} + \frac{|S_{23}|}{3} = n-1$. By (1.2), we get

$$\begin{aligned} RD(u|G) &\leq |S_{21}| + \frac{|S_{22}|}{2} + \frac{|S_{23}|}{3} \\ &= \frac{n-1+deg(u)}{2} - \frac{1}{6} \qquad \text{since } |S_{23}| \geq 1 \\ &= \frac{3n-4+3\deg(u)}{6}. \end{aligned} \tag{3.3}$$

Using (3.2) and (3.3) in (1.3) we get the required result (3.1). □

Theorem 3.2. *Let G be a graph of order n, size m with $diam(G) = rad(G) = 3$, then*

$$H(G) \geq \frac{n^2+4m}{6}. \tag{3.4}$$

Proof. For any vertex $u \in V(G)$ and $diam(G) = rad(G) = 3$, we define the sets $S_{1i} = \{v \in V|1/d(u,v)\}$ for $i = 1,2,3$. Then clearly we can say that, $\left|\bigcup_{i=1}^{3} S_{1i}(u)\right| = n$ and

$$|S_{12}(u)| + |S_{13}(u)| = n - 1 - \deg(u). \tag{3.5}$$

Since $|S_{11}(u)| = \deg(u)$ and $|S_{12}(u)| \geq 2$. Otherwise, there exist a vertex $w \in S_{12}(u)$ such that $e(w) \leq 2$, a contradiction.

Thus, from (1.2) will have the following

$$\begin{aligned} RD(u|G) &= \sum_{v\in V}\frac{1}{d(u,v)} \\ &= |S_{11}(u)| + \frac{|s_{12}(u)|}{2} + \frac{|S_{13}(u)|}{3} \\ &= \deg(u) + \left[\frac{n-1-\deg(u)}{2}\right] - \frac{|S_{13}(u)|}{6}. \qquad (3.6) \\ |S_{13}(u)| &= n-1-\deg(u) - |S_{12}(u)|, \qquad \text{from}(3.5) \\ &\leq n-3-\deg(u), \qquad \because |S_{12}(u)| \geq 2 \end{aligned}$$

Therefore (3.6) becomes,

$$RD(u|G) \geq \frac{n+2\deg(u)}{3}.$$

Using above argument in (1.3), we get the desired result (3.4). □

Remark 3.1. *The upper bound in the Theorem 3.2 is attainable, if $G \cong C_6$.*

Theorem 3.3. *Let G be a graph of order n, size m with $diam(G) = rad(G) = \alpha \geq 3$. Then,*

$$H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2} - n\left[\frac{\alpha-3}{2} - \sum_{i=3}^{\alpha-1}\frac{1}{i} + \frac{(\alpha-2)}{4\alpha}\right]. \qquad (3.7)$$

Equality holds if and only if $G \cong C_{2\alpha}$.

Proof. For any vertex $u \in V(G)$ and $diam(G) = rad(G) = \alpha$, define the sets $S_{1i}(u)$ as $S_{1i}(u) = \{v \in V | 1/d(u,v) = i\}$ for $i = 1,\ 2,\ 3,\ \ldots,\alpha$. Then by the definition of reciprocal distance number we have the following

$$\begin{aligned} RD(u|G) &= |S_{11}(u)| + \frac{|S_{12}(u)|}{2} + \frac{|S_{13}(u)|}{3} + \ldots + \frac{|S_{1\alpha}(u)|}{\alpha} \\ &= \frac{n-1+\deg(u)}{2} - \sum_{i=3}^{\alpha-1}\frac{(i-2)}{2i}(|S_{1i}(u)|) - \frac{\alpha-2}{2\alpha}(|S_{1\alpha}(u)|). \qquad (3.8) \end{aligned}$$

Since $|S_{1i}(u)| \geq 2$, for $i = 1,\ 2,\ 3,\ \ldots \alpha - 1$ and $|S_{1\alpha}(u)| \geq 1$, we get

$$RD(u|G) \leq \frac{n-1+\deg(u)}{2} - 2\sum_{i=3}^{\alpha-1}\left(\frac{i-2}{2i}\right) - \left(\frac{\alpha-2}{2\alpha}\right).$$

Using above argument in (1.3), we get the desired result (3.7).

For the equality, Let $G \cong C_{2\alpha}$ then $diam(G) = rad(G) = \alpha$ and $|S_{1i}(u)| \geq 2$, for $i = 2, 3, \ldots, \alpha - 1$. It is easy to get

$$H(G) = \frac{n(n-1)}{4} + \frac{m}{2} - n\left[\frac{\alpha-3}{2} - \sum_{i=3}^{\alpha-1}\frac{1}{i} + \frac{(\alpha-2)}{4\alpha}\right].$$

Conversely, consider $H(G) = \frac{n(n-1)}{4} + \frac{m}{2} - n\left[\frac{\alpha-3}{2} - \sum_{i=3}^{\alpha-1}\frac{1}{i} + \left(\frac{\alpha-2}{4\alpha}\right)\right]$. We now prove that $G \cong C_{2\alpha}$. Suppose $G \ncong C_{2\alpha}$ then $|S_{1i}(u)| \geq 3$, for $i = 2, 3, \ldots, \alpha - 1$ and by (3.8) we get

$$RD(u|G) \leq \frac{n-1+\deg(u)}{2} - 3\sum_{i=3}^{\alpha-1}\left(\frac{i-2}{2i}\right) - \left(\frac{\alpha-2}{2\alpha}\right). \tag{3.9}$$

Therefore from (3.9), we have

$$H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2} - \frac{3n}{2}\left[\frac{\alpha-3}{2} - \sum_{i=3}^{\alpha-1}\frac{1}{i} + \frac{\alpha-2}{2\alpha}\right]$$

This contradicts to our assumption. Therefore $G \cong C_{2\alpha}$. □

We now give sharp upper bound for Harary index $H(G)$ in terms of vertex connectivity or connectivity which is as follows

Theorem 3.4. *Let G be a graph of order n, connectivity r and $H_1,\ H_2,\ \ldots,\ H_t$ be the connected components of $G - S$, where $|S| = r$.Then,*

$$H(G) \leq \frac{1}{2}\left[l(l+r) + n(n-l-1)\right], \tag{3.10}$$

where $l = \min_{1\leq i\leq t}\{|V(H_i)|\}$. Further, the equality holds if and only if $G = k_1 + k_r + k_{n-l-r}$.

Proof. Let S be any cut set of G with $|S| = r$ and $H_1,\ H_2, \ldots, H_t$ are the connected components of $G - S$ with $l = \min_{1\leq i\leq t}\{|V(H_i)|\}$. Let us assume that $|V(H_i)| = l$, $G_1 = H_1$ and $G_2 = \bigcup_{i=2}^{t} H_i$, then, $|V(G_1)| = l$ and $|V(G_2)| = n - r - l$, and

$$\begin{aligned} H(G) &= \frac{1}{2}\sum_{u\in V} RD(u|G) \\ &= \frac{1}{2}\left[\sum_{u\in V(G_1)} RD(u|G) + \sum_{u\in S} RD(u|G) + \sum_{u\in V(G_2)} RD(u|G)\right]. \end{aligned}$$

Now, consider the following three cases. For any arbitrary vertex in G.

Case (i): Let $u \in V(G_1)$. Then,

$$\begin{aligned} RD(u|G) &= \sum_{v\in V(G)} \frac{1}{d(u,v)} \\ &= \sum_{v\in V(G_1)} \frac{1}{d(u,v)} + \sum_{v\in S} \frac{1}{d(u,v)} + \sum_{v\in V(G_2)} \frac{1}{d(u,v)} \\ &\le (l-1) + r + \frac{n-l-r}{2} \\ &= \frac{n+l+r-2}{2}. \end{aligned}$$

Since $\frac{1}{d(u,v)} \le 1$, if $v \in V(G_1)$, $v \in S$ and $\frac{1}{d(u,v)} \le \frac{1}{2}$, if $v \in V(G_2)$.

Case (ii): Let $u \in S$. Then,

$$\begin{aligned} RD(u|G) &= \sum_{v\in V(G)} \frac{1}{d(u,v)} \\ &= \sum_{v\in V(G_1)} \frac{1}{d(u,v)} + \sum_{v\in S} \frac{1}{d(u,v)} + \sum_{v\in V(G_2)} \frac{1}{d(u,v)} \\ &\le l + r - 1 + n - l - r \\ &= n-1. \end{aligned}$$

Since $\frac{1}{d(u,v)} \le 1$, if v is in either sets $V(G_1)$, S and $V(G_2)$.

Case (iii): Let $u \in V(G_2)$, then we can prove that

$$RD(u|G) \le \left(n - \frac{l}{2} - 1\right).$$

Thus we have,

$$\begin{aligned} H(G) &\le \frac{1}{2}\left\{[n+l+r-2]\frac{l}{2} + (n-1)r + \left(n - \frac{l}{2} - 1\right)(n-l-r)\right\} \\ &= \frac{1}{2}\left\{l(l+r) + n(n-l-1)\right\}. \end{aligned}$$

The second part of the theorem follows from the proof of the inequality itself. □

Remark 3.2. *Our upper bound* (3.10) *is better than the upper bound* (2.1). *We have to show that*

$$(n-1)^2 + r - [l(l+r) + n(n-l-1)] \ge 0,$$

that is

$$n[l-1]-l[l+r]+r+1\geq 0,$$

since $l\geq 1$.

Theorem 3.5. *Let G be any connected graph of order n, then*

$$H(G)\leq \frac{2n(n-1)-\beta_0(\beta_0-1)}{4}.$$

Equality holds if and only if $G=\overline{K}_{\beta_0}+K_{n-\beta_0}$.

Proof. Let us consider a maximum independent set with $|S|=\beta_0$ and $u_i\in S$. Then

$$\begin{aligned} RD(u_i|G) &= \sum_{u_j\in V(G)}\frac{1}{d(u,v)} \\ &= \sum_{u_j\in S}\frac{1}{d(u_i,u_j)}+\sum_{u_j\in V-S}\frac{1}{d(u_i,u_j)} \\ &\leq \frac{1}{2}(\beta_0-1)+n-\beta_0 \\ &= \frac{2n-\beta_0-1}{2}. \end{aligned} \tag{3.11}$$

Since $u_i\neq u_j$ and $u_i\in S$, there are (β_0-1) vertices in S which are at a distance at least two from u_i and $\frac{1}{d(u_i,u_j)}\leq 1$, for any $u_j\in V-S$, then

$$\begin{aligned} RD(u_i|G) &= \sum_{u_j\in V(G)}\frac{1}{d(u,v)}+\sum_{u_j\in S}\frac{1}{d(u_i,u_j)}+\sum_{u_j\in V-S}\frac{1}{d(u_i,u_j)} \\ &\leq \beta_0+n-\beta_0-1 \\ &= n-1. \end{aligned} \tag{3.12}$$

Therefore,

$$\begin{aligned} H(G) &= \frac{1}{2}\left[\sum_{u_j\in S}\frac{1}{d(u_i,u_j)}+\sum_{u_j\in V-S}\frac{1}{d(u_i,u_j)}\right] \\ &\leq \frac{1}{2}\left[\frac{\beta_0}{2}(2n-\beta_0-1)+(n-\beta_0)(n-1)\right] \\ &= \frac{2n(n-1)-\beta_0(\beta_0-1)}{4}, \end{aligned}$$

from (3.11) and (3.12).

Further, if $G = \overline{K}_{\beta_0}+K_{n-\beta_0}$, then easily we can see that $H(G) = \frac{2n(n-1)-\beta_0(\beta_0-1)}{4}$.

Conversely, suppose $H(G) = \frac{2n(n-1)-\beta_0(\beta_0-1)}{4}$. Now, we prove that $G = \overline{K}_{\beta_0} + K_{n-\beta_0}$. If possible assume that $G \neq \overline{K}_{\beta_0} + K_{n-\beta_0}$. Since S be the maximum independent set with $|S| = \beta_0$ in G. For any two vertices in G, $d(u, v) = 2$ if both u and v in S and $d(u, v) = 1$ if both u and v are in $V - S$, otherwise, it will lead to $H(G) < \frac{2n(n-1)-\beta_0(\beta_0-1)}{4}$, a contradiction to our assumption. Hence $< S >= \overline{K}_{\beta_0}$and $< V - S >= K_{n-\beta_0}$. Further, if $u \in S$ and $v \in V - S$, we claim that $\frac{1}{d(u,v)} = 1$, otherwise$\sum_{u\in S} \frac{1}{d(u|G)} < n - \beta_0$ and there by$H(G) < \frac{2n(n-1)-\beta_0(\beta_0-1)}{4}$ holds, a contradiction. Thus $G = \overline{K}_{\beta_0} + K_{n-\beta_0}$ holds. □

Theorem 3.6. *Let G be any connected graph of order n, then*

$$H(G) \leq \frac{2n(n-1) - \gamma_0(\gamma_0 - 1)}{4}.$$

The equality holds if and only if $G = \overline{K}_{\gamma_0} + K_{n-\gamma_0}$.

Proof. The proof techniques of the Theorem 3.6 is same as the Theorem 3.5 □

REFERENCES

[1] F. HARARY: *Grapth Theory*, Narosa Publishing House, New Delhi, 1998.

[2] O. IVANCIUC, T.S. BALABAN, A.T. BALABAN: *Reciprocal distance matrix, related local vertex invariants and topological indices*, J. Math. Chem., **12** (1993), 309–318.

[3] X. LI, Y. FAN: *The connectivity and the Harary index of a graph*, Discrete Appl. Math., **181** (2015), 167–173.

[4] D. PLAVŠIĆ, S. NIKOLIĆ, N. TRINAJSTIĆ, Z. MIHALIĆ: *On the Harary index for the characterization of chemical graphs*, J. Math. Chem., **12** (1993), 235–250.

[5] H.S. RAMANE, V.V. MANJALAPUR: *Some bounds for Harary index of graphs*, Int. J. Sci. Eng. Res., **7**(5) (2016), 26–31.

[6] N. TRINAJSTIĆ, S. NOKOLOIĆ, S.C. BASAK, I. LUKOVITS: *Distance indices and their hyper-counterparts: Intercorrelation and use in the structure-property modeling*, SAR QSAR Environ. Res., **12** (2001), 31–54.

[7] K. XU, K.C. DAS: *Extremal unicyclic and bicyclic graphs with respect to Harary index*, Bull. Malays. Math. Soc., **36**(2) (2013), 373-383.

[8] B. ZHOU, X. CAI, N. TRINAJSTIĆ: *On Harary index*, J. Math. Chem., **44** (2008), 611–618.

DEPARTMENT OF MATHEMATICS
K. L. E. SOCIETY'S, BASAVAPRABHU KORE ARTS, SCIENCE AND COMMERCE COLLEGE, CHIKODI-591201, KARNATAKA, INDIA.
Email address: vinmathsklesbkcc@gmail.com

DEPARTMENT OF MATHEMATICS,
K. L. E. SOCIETY'S, BASAVAPRABHU KORE ARTS, SCIENCE AND COMMERCE COLLEGE, CHIKODI-591201, KARNATAKA, INDIA.
Email address: mahadev17rotti@gmail.com