Harmonic Status Index of Graphs

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Abstract. The status of a vertex u is defined as the sum of the distances between u and all other vertices of a graph G . In this paper we have defined the harmonic status index of a graph and obtained the bounds for it. Further the harmonic status indices of some graphs are obtained.

1. Introduction

Several distance based indices of a graph, such as Wiener index [24], distance energy [13, 18], hyper Wiener index [21], Harary index [14, 17] have been appeared in the literature. In this paper we introduce and study the new index called harmonic status index. Let G be a connected graph of order n and size m . Let $V(G)$ be the vertex set and $E(G)$ be the edge set of G . The edge between the vertices u and v is denoted by uv . The *degree* of a vertex u is the number of edges incident to it and is denoted by $d(u)$. The *distance* between two vertices u and v , denoted by $d(u, v)$, is the length of the shortest u - v path in G . The maximum distance between any pair of vertices in G is called the *diameter* of G and is denoted by $\text{diam}(G)$. For graph theoretic terminology, we refer the books [1, 2].

The *status* [11] of a vertex $u \in V(G)$ is defined as the sum of its distance from every other vertex in $V(G)$ and is denoted by $\sigma(u)$. That is,

$$\sigma(u) = \sum_{v \in V(G)} d(u, v).$$

The *Wiener index* [24] $W(G)$ of a connected graph G is defined as the sum of the distances between all pairs of vertices of G . That is,

$$W(G) = \sum_{\{u, v\} \subseteq V(G)} d(u, v) = \frac{1}{2} \sum_{u \in V(G)} \sigma(u).$$

For more about the Wiener index one can refer [4, 7, 10, 19, 20, 23].

The *harmonic index* of a graph G is defined as [8]

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$

Recent results on the harmonic index can be found in [3, 5, 12, 15, 16, 22, 25, 26]. Inspired by this definition, we define here *harmonic status index* of a connected graph G as

$$HS(G) = \sum_{uv \in E(G)} \frac{2}{\sigma(u) + \sigma(v)},$$

and obtain the bounds for the harmonic status index. Also we obtain the harmonic status index of some graphs. Further the correlation between the boiling point of paraffins and harmonic status index of the corresponding molecular graph is studied.

For a graph given in Fig. 1, $\sigma(u_1) = 5$, $\sigma(u_2) = 3$, $\sigma(u_3) = 4$, $\sigma(u_4) = 4$. And

$$HS(G) = \frac{2}{\sigma(u_1) + \sigma(u_2)} + \frac{2}{\sigma(u_2) + \sigma(u_3)} + \frac{2}{\sigma(u_2) + \sigma(u_4)} + \frac{2}{\sigma(u_3) + \sigma(u_4)} = \frac{15}{14}.$$

Fig. 1. Graph

2. Bounds for the harmonic status index

In this section we obtain the bounds for the harmonic status index of graphs and characterize for the equality of these bounds.

Theorem 1. Let G be a connected graph with n vertices and let $\text{diam}(G) = D$. Then

$$\sum_{uv \in E(G)} \frac{2}{2D(n-1) - (D-1)[d(u) + d(v)]} \leq HS(G) \leq \sum_{uv \in E(G)} \frac{2}{4n-4 - [d(u) + d(v)]}. \quad (1)$$

Equality on both sides holds if and only if $\text{diam}(G) \leq 2$.

Proof. Lower bound: For any vertex u of G , there are $d(u)$ vertices which are at distance 1 from u and the remaining $(n-1-d(u))$ vertices are at distance at most D . Therefore

$$\sigma(u) \leq d(u) + D(n-1-d(u)) = D(n-1) - (D-1)d(u).$$

Therefore $\sigma(u) + \sigma(v) \leq 2D(n-1) - (D-1)[d(u) + d(v)]$. Therefore

$$HS(G) = \sum_{uv \in E(G)} \frac{2}{\sigma(u) + \sigma(v)} \geq \sum_{uv \in E(G)} \frac{2}{2D(n-1) - (D-1)[d(u) + d(v)]}.$$

Upper bound: For any vertex u of G , there are $d(u)$ vertices which are at distance 1 from u and the remaining $(n-1-d(u))$ vertices are at distance at least 2. Therefore

$$\sigma(u) \geq d(u) + 2(n-1-d(u)) = 2n-2-d(u).$$

Therefore $\sigma(u) + \sigma(v) \geq 4n-4 - [d(u) + d(v)]$. Therefore

$$HS(G) = \sum_{uv \in E(G)} \frac{2}{\sigma(u) + \sigma(v)} \leq \sum_{uv \in E(G)} \frac{2}{4n-4 - [d(u) + d(v)]}.$$

For equality: If the diameter D is 1 or 2 then the equality holds.

Conversely, let

$$HS(G) = \sum_{uv \in E(G)} \frac{2}{4n-4 - [d(u) + d(v)]}.$$

Suppose, $D \geq 3$, then there exists at least one pair of vertices u and v such that $d(u, v) \geq 3$. Therefore $\sigma(u) \geq d(u) + 3 + 2(n-2-d(u)) = 2n-1-d(u)$. Therefore

$$HS(G) \leq \sum_{uv \in E(G)} \frac{2}{4n-2 - [d(u) + d(v)]} < \sum_{uv \in E(G)} \frac{2}{4n-4 - [d(u) + d(v)]},$$

a contradiction. Hence $\text{diam}(G) \leq 2$.

Corollary 1.1. Let G be a connected graph with n vertices, m edges and $\text{diam}(G) = D$. Let δ and Δ be the minimum and maximum degree of the vertices of G respectively. Then

$$\frac{m}{D(n-1) - (D-1)\delta} \leq HS(G) \leq \frac{m}{2n-2-\Delta}.$$

Proof. For any vertex u of G , $d(u) \geq \delta$ and $d(u) \leq \Delta$. Therefore substituting $d(u) + d(v) \geq 2\delta$ on left side and $d(u) + d(v) \leq 2\Delta$ on the right side of Eq. (1) we get the result.

Corollary 1.2. Let G be a connected regular graph of degree r with n vertices, m edges and $\text{diam}(G) = D$. Then

$$\frac{m}{D(n-1) - (D-1)r} \leq HS(G) \leq \frac{m}{2n-2-r}.$$

Equality holds if and only if $\text{diam}(G) \leq 2$.

Proof. For any vertex u of G , $d(u) = r$. Therefore the result follows from the Theorem 1.

3. Harmonic status index of some standard graphs

Proposition 2. For a complete graph K_n on n vertices, $HS(K_n) = n/2$.

Proof. For any vertex u of K_n , $\sigma(u) = n-1$. Therefore by the definition of harmonic status index, $HS(K_n) = n/2$.

Proposition 3. For a complete bipartite graph $K_{p,q}$,

$$HS(K_{p,q}) = \frac{2pq}{3(p+q)-4}.$$

Proof. The vertex set $V(K_{p,q})$ can be partitioned into two independent sets V_1 and V_2 such that for every edge uv of $K_{p,q}$, the vertex $u \in V_1$ and $v \in V_2$. Therefore $d(u) = q$ and $d(v) = p$. The graph $K_{p,q}$ has $n = p + q$ vertices and $m = pq$ edges. Also $\text{diam}(K_{p,q}) \leq 2$. Therefore by the equality part of Theorem 1,

$$HS(K_{p,q}) = \sum_{uv \in E(K_{p,q})} \frac{2}{4(p+q)-4-[q+p]} = \frac{2pq}{3(p+q)-4}.$$

Proposition 4. For a path P_n on n vertices,

$$HS(P_n) = \sum_{i=1}^{n-1} \frac{2}{(n-i)^2 + i^2}.$$

Proof. Let $v_1, v_2, \dots, v_n$ be the vertices of P_n , where v_i is adjacent to v_{i+1} , $i = 1, 2, \dots, n-1$. Therefore for $i = 1, 2, \dots, n-1$,

$$\sigma(v_i) = (i-1) + (i-2) + \dots + 1 + 1 + 2 + \dots + (n-i) = \frac{n^2 + n}{2} + i(i-n-1).$$

Therefore

$$HS(P_n) = \sum_{i=1}^{n-1} \frac{2}{\sigma(v_i) + \sigma(v_{i+1})} = \sum_{i=1}^{n-1} \frac{2}{(n-i)^2 + i^2}.$$

Proposition 5. For a cycle C_n on $n \geq 3$ vertices,

$$HS(C_n) = \begin{cases} \frac{4}{n} & \text{if } n \text{ is even} \\ \frac{4n}{n^2 - 1} & \text{if } n \text{ is odd.} \end{cases}$$

Proof. If n is even number then for any vertex u of C_n ,

$$\sigma(u) = 2 \left[1 + 2 + \cdots + \frac{n-1}{2} \right] + \frac{n}{2} = \frac{n^2}{4}.$$

Therefore

$$HS(C_n) = \sum_{uv \in E(C_n)} \frac{2}{\sigma(u) + \sigma(v)} = \frac{4}{n}.$$

If n is odd number then for any vertex u of C_n ,

$$\sigma(u) = 2 \left[1 + 2 + \cdots + \frac{n-1}{2} \right] = \frac{(n^2 - 1)}{4}.$$

Therefore

$$HS(C_n) = \sum_{uv \in E(C_n)} \frac{2}{\sigma(u) + \sigma(v)} = \frac{4n}{n^2 - 1}.$$

A *wheel* W_{n+1} is a graph obtained from the cycle C_n , $n \geq 3$ by adding a new vertex and making it adjacent to all the vertices of C_n . The degree of a central vertex of W_{n+1} is n and the degree of all other vertices is 3.

Fig. 2. Wheel W_7

Proposition 6. For a wheel W_{n+1} , $n \geq 3$,

$$HS(W_{n+1}) = \frac{n(7n-9)}{3(n-1)(2n-3)}.$$

Proof. Partition the edge set $E(W_{n+1})$ into two sets E_1 and E_2 , where $E_1 = \{uv \mid d(u) = n \text{ and } d(v) = 3\}$ and $E_2 = \{uv \mid d(u) = 3 \text{ and } d(v) = 3\}$. It is easy to check that $|E_1| = n$ and $|E_2| = n$. Also $\text{diam}(W_{n+1}) = 2$.

Therefore by the equality part of Theorem 1,

$$\begin{aligned} HS(W_{n+1}) &= \sum_{uv \in E_1} \frac{2}{4(n+1) - 4 - [d(u) + d(v)]} + \sum_{uv \in E_2} \frac{2}{4(n+1) - 4 - [d(u) + d(v)]} \\ &= \frac{n(7n-9)}{3(n-1)(2n-3)}. \end{aligned}$$

A *friendship graph* (or *Dutch windmill graph*) F_n , $n \geq 2$, is a graph that can be constructed by coalescence n copies of the cycle C_3 of length 3 with a common vertex. It has $2n + 1$ vertices and $3n$ edges. The degree of a coalescence vertex of F_n is $2n$ and the degree of all other vertices is 2.

Fig. 3. Friendship graph F_3

Proposition 8. For a friendship graph F_n , $n \geq 2$,

$$HS(F_n) = \frac{n(11n-5)}{(3n-1)(4n-2)}.$$

Proof. Partition the edge set $E(F_n)$ into two sets E_1 and E_2 , where $E_1 = \{uv \mid d(u) = 2n \text{ and } d(v) = 2\}$ and $E_2 = \{uv \mid d(u) = 2 \text{ and } d(v) = 2\}$. It is easy to check that $|E_1| = 2n$ and $|E_2| = n$. Also $\text{diam}(F_n) = 2$.

Therefore, by the equality part of Theorem 1,

$$\begin{aligned} HS(F_n) &= \sum_{uv \in E_1} \frac{2}{4(2n+1) - 4 - [d(u) + d(v)]} + \sum_{uv \in E_2} \frac{2}{4(2n+1) - 4 - [d(u) + d(v)]} \\ &= \frac{n(11n-5)}{(3n-1)(4n-2)}. \end{aligned}$$

4. Harmonic status index of some graphs obtained from the complete graph

In this section we obtain the harmonic status index of the graphs, which were defined in [9].

Proposition 9. Let e_i , $i = 1, 2, \dots, k$, $1 \leq k \leq n-2$, be the distinct edges of a complete graph K_n , $n \geq 3$, all being incident to a single vertex. The graph $Ka_n(k)$ is obtained by deleting e_i , $i = 1, 2, \dots, k$ from K_n . Then

$$HS(Ka_n(k)) = \frac{2(n-k-1)}{2n-2+k} + \frac{k(k-1)}{2n} + \frac{2(n-k-1)k}{2n-1} + \frac{(n-k-1)(n-k-2)}{2n-2}.$$

Proof. The edge set $E(Ka_n(k))$ can be partitioned into four sets E_1 , E_2 , E_3 and E_4 , where $E_1 = \{uv \mid d(u) = n-1-k \text{ and } d(v) = n-1\}$, $E_2 = \{uv \mid d(u) = n-2 \text{ and } d(v) = n-2\}$, $E_3 = \{uv \mid d(u) = n-2 \text{ and } d(v) = n-1\}$ and $E_4 = \{uv \mid d(u) = n-1 \text{ and } d(v) = n-1\}$. It is easy to check that $|E_1| = n-k-1$, $|E_2| = k(k-1)/2$, $|E_3| = (n-k-1)k$ and $|E_4| = (n-k-1)(n-k-2)/2$. Also $\text{diam}(Ka_n(k)) = 2$.

Therefore, by the equality part of Theorem 1,

$$\begin{aligned} HS(Ka_n(k)) &= \sum_{uv \in E_1} \frac{2}{4n-4-[d(u)+d(v)]} + \sum_{uv \in E_2} \frac{2}{4n-4-[d(u)+d(v)]} \\ &\quad + \sum_{uv \in E_3} \frac{2}{4n-4-[d(u)+d(v)]} + \sum_{uv \in E_4} \frac{2}{4n-4-[d(u)+d(v)]} \end{aligned}$$

$$\begin{aligned}
 &= \frac{2(n-k-1)}{2n-2+k} + \frac{2(k(k-1)/2)}{2n} + \frac{2(n-k-1)k}{2n-1} + \frac{2((n-k-1)(n-k-2)/2)}{2n-2} \\
 &= \frac{2(n-k-1)}{2n-2+k} + \frac{k(k-1)}{2n} + \frac{2(n-k-1)k}{2n-1} + \frac{(n-k-1)(n-k-2)}{2n-2}.
 \end{aligned}$$

Proposition 10. Let $f_i, i = 1, 2, \dots, k, 1 \leq k \leq \lfloor n/2 \rfloor$ be independent edges of the complete graph $K_n, n \geq 3$. The graph $Kb_n(k)$ is obtained by deleting $f_i, i = 1, 2, \dots, k$ from K_n . Then

$$HS(Kb_n(k)) = \frac{4k(n-2k)}{2n-1} + \frac{(n-2k)(n-2k-1)}{2n-2} + \frac{2k(k-1)}{n}.$$

Proof. The edge set $E(Kb_n(k))$ can be partitioned into three sets E_1, E_2 , and E_3 , where $E_1 = \{uv \mid d(u) = n-2 \text{ and } d(v) = n-1\}$, $E_2 = \{uv \mid d(u) = n-1 \text{ and } d(v) = n-1\}$, and $E_3 = \{uv \mid d(u) = n-2 \text{ and } d(v) = n-2\}$. It is easy to check that $|E_1| = 2k(n-2k)$, $|E_2| = (n-2k)(n-2k-1)/2$, and $|E_3| = (2k(2k-1)/2) - k$. Also $\text{diam}(Kb_n(k)) = 2$.

Therefore, by the equality part of Theorem 1,

$$\begin{aligned}
 HS(Kb_n(k)) &= \sum_{uv \in E_1} \frac{2}{4n-4-[d(u)+d(v)]} + \sum_{uv \in E_2} \frac{2}{4n-4-[d(u)+d(v)]} + \sum_{uv \in E_3} \frac{2}{4n-4-[d(u)+d(v)]} \\
 &= \frac{2(2k)(n-2k)}{2n-1} + \frac{2((n-2k)(n-2k-1)/2)}{2n-2} + \frac{2((2k(2k-1)/2)-k)}{2n} \\
 &= \frac{4k(n-2k)}{2n-1} + \frac{(n-2k)(n-2k-1)}{2n-2} + \frac{2k(k-1)}{n}.
 \end{aligned}$$

Proposition 11. Let V_k be a k -element subset of the vertex set of the complete graph $K_n, 2 \leq k \leq n-1, n \geq 3$. The graph $Kc_n(k)$ is obtained by deleting from K_n all the edges connecting pairs of vertices from V_k . Then

$$HS(Kc_n(k)) = \frac{2k(n-k)}{2n+k-3} + \frac{(n-k)(n-k-1)}{2n-2}.$$

Proof. The edge set $E(Kc_n(k))$ can be partitioned into two sets E_1 , and E_2 , where $E_1 = \{uv \mid d(u) = n-k \text{ and } d(v) = n-1\}$ and $E_2 = \{uv \mid d(u) = n-1 \text{ and } d(v) = n-1\}$. It is easy to check that $|E_1| = (n-k)k$ and $|E_2| = (n-k)(n-k-1)/2$. Also $\text{diam}(Kc_n(k)) = 2$.

Therefore, by the equality part of Theorem 1,

$$\begin{aligned}
 HS(Kc_n(k)) &= \sum_{uv \in E_1} \frac{2}{4n-4-[d(u)+d(v)]} + \sum_{uv \in E_2} \frac{2}{4n-4-[d(u)+d(v)]} \\
 &= \frac{2(n-k)k}{2n+k-3} + \frac{2((n-k)(n-k-1)/2)}{2n-2} \\
 &= \frac{2k(n-k)}{2n+k-3} + \frac{(n-k)(n-k-1)}{2n-2}.
 \end{aligned}$$

Proposition 12. Let $3 \leq k \leq n, n \geq 5$. The graph $Kd_n(k)$ is obtained by deleting from K_n , the edges belonging to a k -membered cycle. Then

$$HS(Kd_n(k)) = \frac{k(k-3)}{2n+2} + \frac{k(n-k)}{n} + \frac{(n-k)(n-k-1)}{2n-2}.$$

Proof. The edge set $E(Kd_n(k))$ can be partitioned into three sets E_1 , E_2 and E_3 , where $E_1 = \{uv \mid d(u) = n - 3 \text{ and } d(v) = n - 3\}$, $E_2 = \{uv \mid d(u) = n - 3 \text{ and } d(v) = n - 1\}$ and $E_3 = \{uv \mid d(u) = n - 1 \text{ and } d(v) = n - 1\}$. It is easy to check that $|E_1| = (k(k - 1)/2) - k$, $|E_2| = (n - k)k$ and $|E_3| = (n - k)(n - k - 1) / 2$. Also $\text{diam}(Kd_n(k)) = 2$.

Therefore by the equality part of Theorem 1,

$$\begin{aligned} HS(Kd_n(k)) &= \sum_{uv \in E_1} \frac{2}{4n - 4 - [d(u) + d(v)]} + \sum_{uv \in E_2} \frac{2}{4n - 4 - [d(u) + d(v)]} + \sum_{uv \in E_3} \frac{2}{4n - 4 - [d(u) + d(v)]} \\ &= \frac{2((k(k - 1)/2) - k)}{2n + 2} + \frac{2k(n - k)}{2n} + \frac{2((n - k)(n - k - 1)/2)}{2n - 2} \\ &= \frac{k(k - 3)}{2n + 2} + \frac{k(n - k)}{n} + \frac{(n - k)(n - k - 1)}{2n - 2}. \end{aligned}$$

Note that $HS(Kd_4(3)) = 3/4$ and the graphs $Kd_3(3)$ and $Kd_4(4)$ are disconnected.

5. Correlation between harmonic status index and boiling point of paraffins

The properties of graphs can be used in the study of quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) of the molecules [6]. In this section we study the correlation between the boiling point (BP) of the paraffin hydrocarbons and the harmonic status index of the corresponding molecular graphs.

Table 1. Boiling point and harmonic status index of paraffins

Paraffin	Boiling point (BP) °C	Harmonic status index (HS)
3-methylpentane	62.9	0.542
2,2 -dimethylbutane	50	0.653
2,3 dimethylbutane	57.9	0.587
2,2 dimethylpentane	79	0.517
3,3 dimethylpentane	86	0.549
n-octane	125	0.4226
3-methylheptane	118	0.406
3-ethylhexane	118	0.4351
2,2-dimethylhexane	107	0.44401
2,4 dimethylhexane	108	0.4386
2-methyl, 3-ethylpentene	116	0.4535
2,2,4-trimethylpentene	99	0.4779
n-dodecane	216.2	0.283

Using the data of Table 1, the scatter plot between the boiling point (BP) and harmonic status index (HS) of paraffins is depicted in Figure 4.

Fig. 4. Regression line between the boiling point (BP) and the harmonic status index (HS) of paraffins

The linear regression between BP and HS is $BP = 306.8(\pm 21.742) - 426.1(\pm 44.741)HS$.

The correlation of the boiling point of paraffins with the harmonic status index is good ($R = 0.9444$).

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