On Harmonic Index Some Special Graphs with Certain Vertex Gluing Graphs

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Abstract: *The stability of cycloalkanes strain energy, branched alkanes and linear alkanes, can be reasonably modeled using the harmonic index (H), which is commonly defined as* $H(G) = \sum_{u-v} \frac{2}{d(u)+d(v)}$ *where d(u) denotes the vertex degree of u in graph G. In the current work, public equation is derived to the H index of vertex gluing and certain graphs.*

Keywords: Harmonic index ,Vertex Gluing.

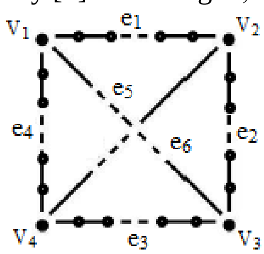
1. Introduction

Characteristics of molecules can be physically/chemically modeled using tools called topological indices, which have the potentials to design the active pharmacological compounds, recognize the environmentally dangerous materials, etc. [2]. Therefore, authors have been attracted to present a variety of researches on such indices, to name a few. The harmonic index, which is considered of great importance, is utilized in modeling the branching of alkanes skeleton that includes carbon-atom. In the 1980s, a computer code to model the automatic generation of conjectures was established by Siemion Fajtlowicz using graph theory, where the likely relations between countless graph invariants, including the vertex-degree-based, were investigated [10-11]. Subsequently, however, no considerable attention has been paid for the H(G) predicted, especially by the chemists. So far, this quantity has not been reintroduced until 2012, when Zhang introduced it as a “harmonic index”, which has recently attracted many researchers to readopt this methodology. For example, the harmonic index was successfully employed in chemical applications, but, knowing the present situation in mathematical chemistry, such authors are very much to be expected [1], [3-6], [9].

In this theory, the graph is symbolized as G=(V,E), where $V = \{v_1, . . . , v_{n-1}, v_n\}$ is the vertex set, while E=E(G) is the edge set of G. Assuming that $v_iv_j \in E$, hence, $G - v_iv_j$ can be denote to left graph G after cancelling the edge vivj. In a molecular graph, the valence of a molecule, i.e. bonds number on a vertex, is represented by the degree of each vertex. In case that d(v) equals to unity, v is said to be a pendent vertex. Moreover, the edge being incident to a pendent vertex is known as a pendent edge. Finally, a chemical is that sort of trees with maximal vertex degree does not exceed 4 [7].

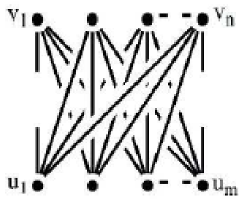
2. Basic Definitions and known Results

“A K_4 –homeomorphism graph is the graph obtained when the six edges of a complete graph with four vertices (K_4) are subdivided into (e_1, e_2, e_3, e_4, e_5, e_6) segments, respectively [8] ” see “Fig. 1,”.



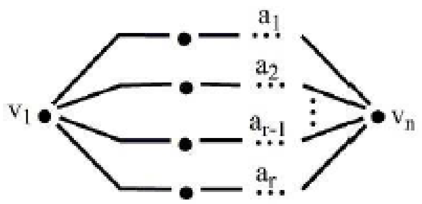
“Fig. 1. (K_4) – homeomorphism graph”

"A complete bipartite graph is a simple bipartite graph with partite sets V_1 and V_2, where every vertex in V_1 is adjacent with all vertices in V_2. If $|V_1|$=n and $|V_2|$=m, then such complete bipartite graph is denoted by $K_{n,m}$ or (K (n,m)). So $K_{n,m}$ has order (n+m) and size (nm). A tree $K_{1,m}$ is also called a star [8]" see "Fig. 2,".



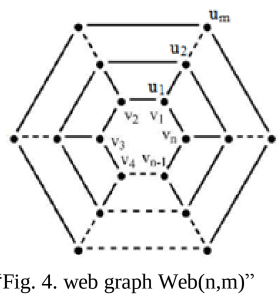
"Fig. 2. complete bipartite graph"

"A (r) – bridge graph is a graph consisting of s paths joining two vertices, which is denoted by Q(a_1,……..,a_r), where a_1,…….,a_r , are the lengths of r paths [8]" see "Fig. 3,".



"Fig. 3. (r) – bridge graph"

"A web graph Web(n,m) is the graph obtained from the Cartesian product of the cycle C_n and the path P_m [8]" see "Fig. 4,".



"Fig. 4. web graph Web(n,m)"

Firstly, examples of some simple graphs are solved for the harmonic index.

Lemma 2.1.

Let K_n is a complete graph of order n, then the harmonic index, $H(K_n) = \frac{n}{2}$.

Lemma 2.2.

Let C_n be a cycle of order n, n ≥3 and size m (n=m), then the harmonic index of C_n is, $H(C_n) = \frac{n}{2}$.

Lemma 2.3.

Let S_n be a star of order n, then the harmonic index of S_n, $H(S_n) = \frac{2(n-1)}{n}$.

Lemma 2.4.

Let P_n be a path of order n, then the harmonic index of a path P_n is as follows:

1- When n=2 then $H(P_1) = 1$.

2- When n=3 then $H(P_3) = \frac{4}{3}$.

3. When n≥4 then $H(P_n) = \frac{4}{3} + \frac{1}{2}(n-3)$

3. The Harmonic Index of Some Special Graphs

Theorem 3.1.

Let e_1, e_2, e_3, e_4, e_5 and e_6 be positive integers. The harmonic index of k_4-homeomorphim graph is denoted by $K_4(e_1, e_2, e_3, e_4, e_5, e_6)$ as follows:

1- If e_1, e_2, e_3, e_4, e_5 and e_6 =1, then the H-index of K_4 – homeomorphism is 2 .

2- If e_1,e_2,e_3,e_4,e_5 and e_6 ≠1 such that e_i ,(i=1,….,6) have k vertices in every e_i, then the H-index of K_4– homeomorphism is $\frac{24}{5} + 3(k-1)$

Proof:

1- If e_1,e_2,e_3,e_4,e_5 and e_6 =1, thus each of them has two vertices of the same third degree besides only one edge. Thus, the H – index will be:

H(K_4–homeomorphism)

$$= \sum_{u-v} \frac{2}{d(u)+d(v)}$$

$$= 6 \cdot \frac{2}{3+3} = 2$$

2- If e_1, e_2, e_3, e_4, e_5 and e_6 ≠1 see "Fig. 1," then each one of them has two or more edges having three degrees for their vertices located at the terminals and only two degrees for the remaining vertices. Therefore, every e_i (i=1,…,6) will have(k –1) edge; and hence, all remaining (k –3) edges will be of the same two degree. So, we have $6(k-3)\frac{2}{2+2}$ edges.

That is,

$$H(K_4(e_1,e_2,e_3,e_4,e_5,e_6)) = 12\cdot\frac{2}{2+3}+\frac{12}{4}(k-3)$$

$$=\frac{24}{5}+3(k-3)$$

Theorem 3.2.

If n, m are positive integers, then the harmonic index of a web graph is denoted by web (n, m) as follows:

1- If m=2 then, $H(web(n,2)) = n$.

2- If m=3 then, $H(web(n,3)) = \frac{125n}{84}$.

3- If m ≥4, then $H(web(n,m)) = \frac{n[42m-1]}{84}$.

Proof:

1- When m=2 and n≥3, then the web (n,2) is obtained from the Cartesian product of the C_n and P_2 see "Fig. 5 (a),". Thus, we have 2n edges, where each one of them have two vertices. Then, $d(v_i)=3$; (i=1,2). Since every path in the web graph is incident with the vertex of C_n of n≥3, then we have n paths with one edge for each of them, So, we have n edges with two vertices for each one of them, where every vertex $d(u_i)=3$; (i=1,2). Hence, by the definition of harmonic index:

$$H(web(n,2)) = 2n\frac{2}{3+3}+n\frac{2}{3+3}=\frac{4n+2n}{6}=n$$

2- When m=3 and n≥3 then web (n,3) is obtained from (C_n) and (P_3) see "Fig. 5.(b),". So, we have 2n edges obtained from the edges of first cycle and third cycle, where each one of them have two vertices. Thus, $d(v_i)=3$; (i=1,2). If we have (n) edges (the number of edges for the second cycle), where each one of them have two vertices $d(v_i) = 4$; (i=1,2). Also, we have n paths, each path have 2 edges with two vertices for each edge, then, $d(u_1) = 3$ and $d(u_2) = 4$. Hence, by definition of harmonic index:

$$H(web(n,2)) = 2n\frac{2}{3+3}+n\frac{2}{4+4}+2n\frac{2}{3+4} = \frac{125n}{84}$$

3- When m ≥ 4 and n ≥ 3, then the web (n,m) is the web graph calculated from C_n and P_m see "Fig. 5 (c),". Thus, we have (2n) edges obtained from the edge of first cycle and final cycle, where each one of them have two vertices as $d(v_i) = 3$; (i=1,2). Then, (m-2)n edges of the total number of cycle edges "excluding the first and final cycles" will have two vertices with $d(v_i) = 4$; (i=1,2). Also, we have n paths with (m-1) edges for each of them, where two edges in every path are incident with two vertices of degree 3 and 4. Thus, $d(u_1)=3$ and $d(u_2)=4$. Moreover, m-3 edges in every path are incident with two vertices of degree 3; that is $d(u_i)=3$ and (i=1,2). subsequently, the harmonic index definition is,

$$H(web(n,m)) = 2n\frac{2}{3+3}+(m-2)n\frac{2}{4+4}+2n\frac{2}{3+4}$$

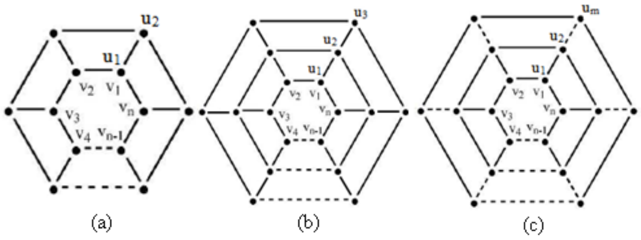
$$+(m-3)n\frac{2}{4+4}$$

$$H(web(n,m)) = \frac{2n}{3}+\frac{2n(m-2)}{8}+\frac{4n}{7}+\frac{n(m-3)}{4}$$

$$=\frac{2n}{3}+\frac{nm}{8}-\frac{n}{2}+\frac{4n}{7}+\frac{nm}{4}-\frac{3n}{4}$$

$$=\frac{56n-42n-63n+18}{84}+\frac{1}{2}nm$$

$$=\frac{-n}{84}+\frac{nm}{2}=\frac{42nm-n}{84}=\frac{n[42m-1]}{84}$$



"Fig. 5. Web graph web(n,m)"

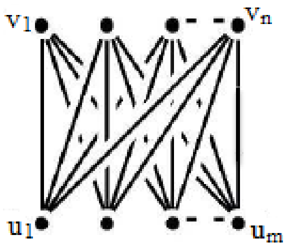
Theorem 3.3.

Suppose that n, m are positive integers, then the complete bipartite graph, which is denoted by $(k_{n,m})$, will have a harmonic index of $H(K_{n,m}) = \frac{2nm}{n+m}$

Proof:

If we have a number of edges nm, where every one of these edges has couple of vertices having equal degree see "Fig. 6,". i.e. m and n are respectively the degree of first and second vertex. Hence, by definition of harmonic index, we get

$$H(K_{n,m})=\sum_{u-v}\frac{2}{d(u)+d(v)}=nm\frac{2}{n+m}=\frac{2nm}{n+m}$$



"Fig. 6. complete bipartite graph"

Theorem 3.4.

Let $Q(a_1,a_2,\ldots\ldots,a_k)$ be a k – Bridge graph, (k) is a positive integer, and n is the number of vertices for any path. Then, the harmonic index of the k – Bridge is:

$$H(Q(a_1,a_2,\ldots,a_k))=\frac{4k}{k+2}+\frac{k}{2}(n-3)$$

Proof:

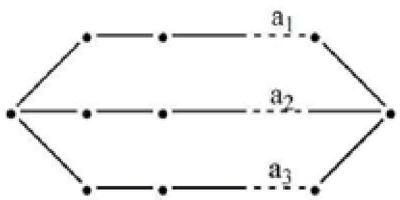
Let k=3, then the graph $G=Q(a_1,a_2,a_3)$ is as shown in "Fig. 7," : Thus,

$$H(Q(a_1,a_2,a_3))=\frac{12}{5}+\frac{3}{2}(n-3)$$

Hence, it is true with,

$$H(Q(a_1,a_2,\ldots,a_k))=\frac{4k}{k+2}+\frac{k}{2}(n-3)$$

$$=\frac{4\cdot 3}{3+2}+\frac{3}{2}(n-3)=\frac{12}{5}+\frac{3}{2}(n-3)\text{; when k=3.}$$



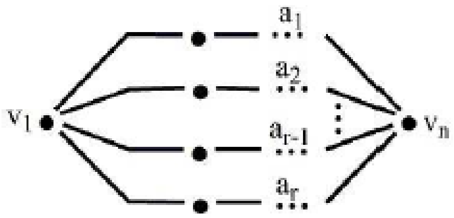
"Fig. 7. (3) – Bridge graph $Q(a_1,a_2,a_3)$"

Assuming that this theory is valid for k = r (r ≥ 3), then the H-index for $Q(a_1,a_2,\ldots,a_r)$ is given by:

$$H(Q(a_1,a_2,\ldots,a_r))=\frac{4r}{(r+2)}+\frac{r}{2}(n-3)\ .$$

Constructing the graph (Q_{r+1}) as follows, $Q(a_1,a_2,\ldots,a_r)$ has the sample:

Where the location of the edges represents a_1 included within graph $Q(a_1,a_2,\ldots,a_r)$ at the i^{th} position see "Fig. 8,".

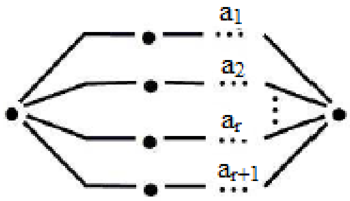


"Fig. 8. (r) – Bridge graph"

The graph U is the path that contains terminals u_1 and u_n, where n is the number of vertices in U as follows see "Fig. 9,".

"Fig. 9. Path"

Connecting the graph $Q(a_1,a_2,\ldots,a_r)$ with the graph (U) such that $v_1 = u_1$ and $v_n = u_n$, then, the vertices $v_1=u_1$ and $v_n = u_n$ are of degree (r+1) see "Fig. 10,".



"Fig. 10. (r+1) – Bridge graph"

Thus,

$$H(Q_{r+1})=\frac{4r}{(r+1)+2}+\frac{r}{2}(n-3)+\frac{4}{(r+1)+2}+(n-3)\cdot\frac{1}{2}$$

$$H(a_1,a_2,\ldots,a_{r+1})=\frac{4}{(r+3)}(r+1)+\frac{n-3}{2}(r+1)\ ,$$

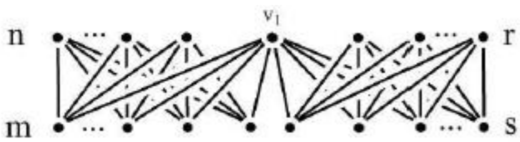
Since (k=r+1)

$$H(a_1,a_2,\ldots,a_{r+1})=\frac{4k}{k+2}+\frac{k}{2}(n-3)$$

$$=\frac{4k}{k+2}+\frac{k}{2}(n-3)$$

4. The Harmonic Index of Certain Vertex Gluing Graphs

"Let v_1–gluing of Complete bipartite graph be a graph obtained from two different Complete bipartite graphs $K_{n,m}$ and $K_{h,t}$ with common one vertex $v_1$denoted by $K_{n,m}^{h,t}(v_1)$ (vertex gluing of graph) [8]", see "Fig. 11,"



"Fig. 11. (v_1) − gluing of Complete bipartite graph"

Theorem 4.1.

Suppose that n, m, h and t are positive integers, then, the v_1– gluing of a complete bipartite graph H –index $K_{n,m}^{h,t}(v_1)$ is:

$$H(K_{n,m}^{h,t}(v_1)) = \frac{2m(n-1)}{(n+m)} + \frac{2t(h-1)}{(h+t)} + \frac{2m}{(n+m+t)} + \frac{2t}{(h+m+t)}$$

Proof:

We have two complete bipartite graphs connected with a common vertex, where every one of them has H – index $\frac{2nm}{n+m}$ by using Theorem 3.3. Thus,

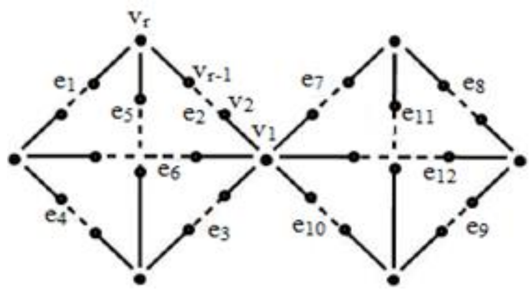
deleting the H – index of the m edges connected with v_1– gluing equals to ($m\frac{2}{n+m}$). On the other hand, adding the H–index of the m edges equals to ($m\frac{2}{n+(m+t)}$). Thus, every edge have degrees of n and (m+t), when (m+t) is the degree of vertex v_1 – gluing. So,

$$H(K_{n,m}^{h,t}(v_1)) = \frac{2nm}{(n+m)} - m\frac{2}{(n+m)} + m\frac{2}{n+(m+t)} + \frac{2ht}{(h+t)} - t\frac{2}{(h+t)} + t\frac{2}{h+(m+t)}$$

$$= (nm-m)\frac{2}{(n+m)} + (ht-t)\frac{2}{(h+t)} + \frac{2m}{n+(m+t)} + \frac{2t}{h+(m+t)}$$

$$= \frac{2m(n-1)}{(n+m)} + \frac{2t(h-1)}{h+t} + \frac{2m}{n+m+t} + \frac{2t}{h+m+t} \quad ■$$

"Let K_4^2 – homeomorphism be a graph obtained from two deferent K_4 – homeomorphism graphs $K_4(e_1, e_2, e_3, e_4, e_5, e_6)$ and $K_4(e_7, e_8, e_9, e_{10}, e_{11}, e_{12})$, with common one vertex v_1 (vertex gluing of graph) [8]", see "Fig. 12,".



"Fig. 12. K_4^2 – homeomorphism graph"

Theorem 4.2.

Let e_i be a positive integer such that $1 \le i \le 12$ and every e_i has k vertices and an edge length of (k–1), then the harmonic index of the K_4^2 – homeomorphism graph is:

1- If length of e_i =1 then,

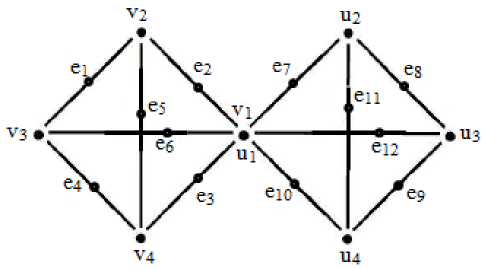
$$H(K_4^2 - homeomorphism) = \frac{10}{3}.$$

2- If length of e_i =2 see "Fig. 13," then,

$$H(K_4^2 - homeomorphism) = \frac{87}{10}.$$

3- If length of e_i =k-1 , $k \ge 4$ then,

$$H(K_4^2 - homeomorphism) = \frac{87}{10} + 6(k-3).$$



"Fig. 13. K_4^2 – homeomorphism graph (e_i =2)"

Proof:

1- By using the definition, $\sum \frac{2}{d(u)+d(v)} = \frac{10}{3}$

2- By using the definition then,

$$H(K_4^2 - homeomorphism) = \frac{87}{10}$$

3- We prove that by mathematical indication:
If k =4, then the length of e_i =3. Using the definition, we get $H(K_4^2 - homeomorphism) = \frac{147}{10}$

It is true that,

$$H(K_4^2 - homeomorphism) = \frac{87}{10} + 6(k-3)$$

$$= \frac{87}{10} + 6(4-3) = \frac{147}{10}$$

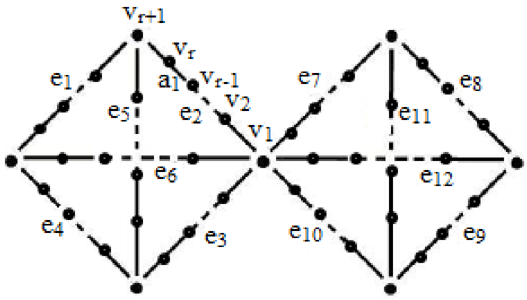
Assuming that this is true for $r \ge 4$ see "Fig. 12," so,

$$H(K_4^2 - homeomorphism) = \frac{87}{10} + 6(r-3).$$

To prove this is true for k =r+1, a one vertex is added for all, i.e. e_i, i =1, 2, ..., 12. So, the number of edges is increased (1) in every e_i, that is we have a new edge a_i in every e_i see "Fig. 14,"). Two vertices for a_i have 2 degrees, and we have 12 edges for K_{42} –homeomorphism. Hence, we add $12.\frac{2}{2+2}$ for $\frac{87}{10}+6(r-3)$, that is,

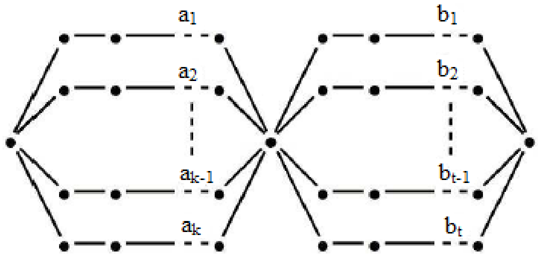
$$H(K_4^2-\text{homeomorphism})=\frac{87}{10}+6(r-3)+12\frac{2}{2+2}$$
$$=\frac{87}{10}+6(k-3)+6$$

$=\frac{87}{10}+6[r-3+1]$ since k=r+1, $=\frac{87}{10}+6[k-3]$



"Fig. 14: K_4^2 – homeomorphism graph (e_i =1,2,…,r+1)"

"Let v_1–gluing of k,t – Bridge graph be a graph obtained from two different k – Bridge graph Q_1 and t-Bridge graph Q_2 with common vertex v_1 denoted by Q_k^t (v_1)(vertex gluing of graph) [8]", see "Fig. 15,".



"Fig. 15. (v_1) – gluing of (k,t) – Bridge graph"

Theorem 4.3.

Let k, t, s and h be positive integers. Then, the v_1 – gluing of k ,t – Bridge graph of H – index Q_k^t (v_1) is:

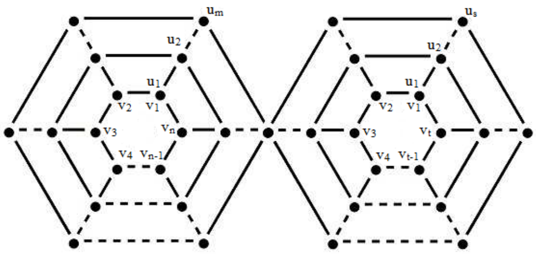
$$H(Q_k^t(v_1))=\frac{2k}{k+2}+\frac{2t}{t+2}+\frac{2(k+t)}{k+t+2}+\frac{k(n-3)}{2}+\frac{t(h-3)}{2}$$

Proof:

We have two k– Bridge graph connected with common vertex v_1 see "Fig. 15," and every vertex of them have H–index $\frac{4k}{k+2}+\frac{k(n-3)}{2}$. By Theorem 3.4, deleting the H–index for k edges connected with v_1–gluing deleting $k\frac{2}{k+2}$, and adding the H–index of k edges $k\frac{2}{2+(k+t)}$ that is every edge have degree 2 and (k+t), where (k+t) is the degree of the vertex v_1 – gluing. Similarly to what followed with t – Bridge,

$$H(Q_k^t(v_1))=\frac{4k}{k+2}+\frac{k(n-3)}{2}+\frac{4t}{t+2}+\frac{t(h-3)}{2}$$
$$-\frac{2k}{t+2}-\frac{2t}{t+2}+\frac{2k}{(k+t)+2}+\frac{2t}{(k+t)+2}$$
$$=\frac{2k}{k+2}+\frac{2k}{k+t+2}+\frac{k(n-3)}{2}+\frac{2t}{t+2}+\frac{2t}{k+t+2}+\frac{t(h-3)}{2}$$
$$=\frac{2k}{k+2}+\frac{2t}{t+2}+\frac{2(k+t)}{k+t+2}+\frac{k(n-3)}{2}+\frac{t(h-3)}{2}$$

"Let v_1 – gluing of web graph be a graph obtained from two different web graphs web (n,m) and web(s,t) with one common vertex v_1 denoted by $W_{n,m}^{s,t}(v_1)$ (vertex gluing of graph) [8]" see "Fig. 16,".



"Fig. 16. v_1- gluing of web graph"

Theorem 4.4.

Let (n, m, s and t) be positive integers. Then, the v_1–gluing of web graph of H–index $W_{n,m}^{s,t}(v_1)$ is:

1. If m, s =2 and n, t ≥ 3 then,
   $$H(W_{n,2}^{t,2}(v_1))=n+t-\frac{2}{3}$$
2. If m, s =3 and n, t ≥ 3 then,
   $$H(W_{n,3}^{t,3}(v_1))=\frac{125}{84}(n+t)-\frac{194}{315}$$
3. If m, s ≥ 4 and n, t ≥ 3 then,
   $$H(W_{n,m}^{t,s}(v_1))=\frac{3n[42m-1]+3t[42s-1]-168}{84}$$

Proof:

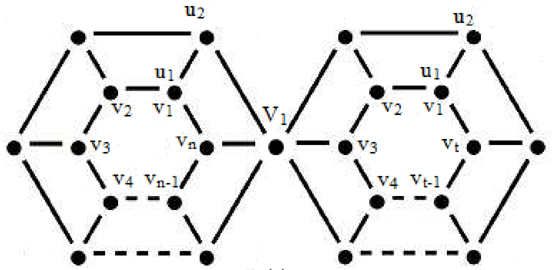
We have two web graphs connected with a common vertex v_1, where every vertex of them has an H–index as:

1- $H(web(n,2)) = n$ by Theorem 3.2 (1), we delete $3.\frac{2}{3+3}$, which are the edges connected with v_1, and we add $3.\frac{2}{3+6}$, which are the edges connected with v_1–gluing see "Fig. 17 (a),". Similarly, work to $H(web(t,2))$ so,

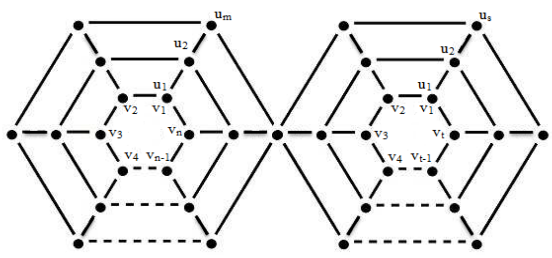
$$H(W_{n,2}^{t,2}(v_1)) = n + t - \frac{2}{3} = n - 3.\frac{2}{3+3} + 3.\frac{3}{3+6} + t - 3.\frac{2}{3+3} + 3.\frac{3}{3+6} = n + t - \frac{2}{3}$$

This proof is similar to proof (1), but one of the deleted edges has 3 degrees on one vertex and 4 on the other vertex, while one of the added edges has (4) degrees on one vertex and 6 on the other vertex see "Fig. 17 (b),". We use Theorem 3.2 (2).

$$H(W_{n,3}^{t,3}(v_1)) = n + t - \frac{2}{3} = \frac{125n}{84} + \frac{125t}{84} - 2\frac{2}{3+4} - 4\frac{2}{3+3} + 2\frac{2}{6+4} + 4\frac{2}{6+3} = \frac{125(n+t)}{84} - \frac{194}{315}$$



(a)



(b)

Fig. 17. v_1- gluing of web graph $web(t,2)$, and $web(t,3)$

3- This proof is similar to proof (2) and by Theorem 3.2 *(3)* then,

$$H(W_{n,m}^{t,s}(v_1)) = \frac{n[42m-1]}{84} + \frac{t[42s-1]}{84} - \frac{194}{315}$$

$$= \frac{(n+t)[42m-1+42s-1]}{84} - \frac{194}{315}$$

$$= \frac{(n+t)[42(m+s)-2]}{84} - \frac{194}{315}$$

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