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(RECOMMENDED CITATION)

ON SOME TOPOLOGICAL INDICES OF THE GENERALIZED HIERARCHICAL PRODUCT OF GRAPHS

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ABSTRACT. The generalized hierarchical product of graphs was introduced very recently by L. Barriére et al. In this paper, revised Szeged and new version of Zagreb indices of generalized hierarchical product of two connected graphs are obtained. Using the results obtained here, some known results are deduced as corollaries. Finally, we obtain the Sz^*, M^*_1 and M^*_2 indices of the zig-zag polyhex nanotube $TUHC_6[2n, 2]$, linear phenylene F_n, hexagonal chain L_n and truncated cube as a consequence of our results.

Keywords: *Generalized hierarchical product, Cartesian product, Revised Szeged index, Zagreb indices.*

INTRODUCTION

Throughout this paper all graphs considered are finite, simple and connected. The **distance** $d(u,v)$ between the vertices u and v of a graph G is equal to the length of a shortest path that connects u and v. Suppose G is a graph with vertex and edge sets $V = V(G)$ and $E = E(G)$, respectively. Suppose $e = uv \in E(G)$. The set of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $N_u^G(e)$. In addition, let $N_0^G(e)$ denote the set of vertices with equal distances to u and v. The **Szeged** and **revised Szeged indices** of the graph G are defined as:

$$Sz(G) = \sum_{e=uv\in E(G)} |N_u^G(e)||N_v^G(e)| \text{ [1, 2, 3]},$$

$$Sz^*(G) = \sum_{e=uv\in E(G)} \left(|N_u^G(e)| + \frac{|N_0^G(e)|}{2}\right)\left(|N_v^G(e)| + \frac{|N_0^G(e)|}{2}\right) \text{ [4, 5, 6]}.$$

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The **Zagreb indices** have been introduced by Gutman and Trinajstic as $M_1(G) = \sum_{u\in V(G)} (deg_G(u))^2$ and $M_2(G) = \sum_{uv\in E(G)} deg_G(u)deg_G(v)$, where $deg_G(u)$ denotes the degree of vertex u [7, 8]. In [9], a new version of Zagreb indices were defined as $M_1^*(G)=\sum_{uv\in E(G)}[\varepsilon_G(u)+\varepsilon_G(v)]$, $M_1^{**}(G)= \sum_{u\in V(G)} (\varepsilon_G(u))^2$ and $M_2^*(G)=\sum_{uv\in E(G)} \varepsilon_G(u)\varepsilon_G(v)$, where $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of G. The total connectivity index $\zeta(G)$ of a graph G is defined as $\zeta(G)= \sum_{u\in V(G)} \varepsilon_G(u)$, see [10].

A graph G with a specified vertex subset $U \subseteq V(G)$ is denoted by $G(U)$. Suppose G and H are graphs and $U \subseteq V(G)$. The **generalized hierarchical product**, denoted by $G(U) \Pi H$, is the graph with vertex set $V(G) \times V(H)$ and two vertices (g, h) and (g', h') are adjacent if and only if $g = g' \in U$ and $hh' \in E(H)$ or, $gg' \in E(G)$ and $h = h'$, see Figure 1. This graph operation introduced recently by Barriere et al. [11, 12] and found some applications in computer science. The **Cartesian product**, $G \times H$, of graphs G and H has the vertex set $V(G\times H) =V(G) \times V(H)$ and $(u, x)(v, y)$ is an edge of $G \times H$ if $u = v$ and $xy\in E(H)$ or, $uv \in E(G)$ and $x = y$ [13, 14].

We denote by P_n and C_n the path and cycle with n vertices, respectively. A bipartite graph is a graph whose vertices can be partitioned into two disjoint subsets U_1 and U_2 such that every edge connects a vertex in U_1 to one in U_2; that is, U_1 and U_2 are independent sets. Our other notations are standard and taken mainly from the standard books of graph theory.

RESULTS AND DISCUSSION

We first introduce some notations. Let $G = (V, E)$ be a graph and $U \subseteq V$. In $G(U)$, an u–v path through U is an u–v path in G containing some vertex $w \in U$ (vertex w could be the vertex u or v). Let $d_{G(U)}(u,v)$ denote the length of a shortest u–v path through U in G. Notice that, if one of the vertices u and v belong to U, then $d_{G(U)}(u,v) = d_G(u,v)$. Furthermore, let $\varepsilon_{G(U)}(u) = \max\{ d_{G(U)}(v, u) \mid v \in V(G(U))\}$, then $\zeta(G(U))$, $M_1^*(G(U))$, $M_2^*(G(U))$ and $M_1^{**}(G(U))$ can be defined as follows:

$$\zeta(G(U))= \sum_{u\in V(G(U))} \varepsilon_{G(U)}(u),\quad M_1^*(G(U))= \sum_{uv\in E(G(U))} [\varepsilon_{G(U)}(u)+\varepsilon_{G(U)}(v)],$$

$$M_1^{**}(G(U))= \sum_{u\in V(G(U))} (\varepsilon_{G(U)}(u))^2 \text{ and}$$

$$M_2^*(G(U)) = \sum_{uv \in E(G(U))} \varepsilon_{G(U)}(u)\varepsilon_{G(U)}(v).$$

For an edge $e = ab$ of $G(U)$, $N_a^{G(U)}(e)$ denotes the set of vertices closer to a than b through U in G and $N_0^{G(U)}(e)$ denotes the set of equidistant vertices of e through U in $G(U)$, i.e.

$$N_a^{G(U)}(e) = \{ u \in V(G(U)) \mid d_{G(U)}(u,a) < d_{G(U)}(u,b)\},$$
$$N_0^{G(U)}(e) = \{ u \in V(G(U)) \mid d_{G(U)}(u,a) = d_{G(U)}(u,b)\}.$$

Then $Sz^*(G(U))$, $Sz^{**}(G(U))$ and $Sz^{***}(G(U))$ can be defined as follows:

$$Sz^*(G(U)) = \sum_{e=uv \in E(G)} \left(|N_u^{G(U)}(e)| + \frac{|N_0^{G(U)}(e)|}{2}\right)\left(|N_v^{G(U)}(e)| + \frac{|N_0^{G(U)}(e)|}{2}\right),$$

$$Sz^{**}(G(U)) = \frac{1}{2}\sum_{e=uv \in E(G(U))} \left(|N_u^{G(U)}(e)||N_v^{G}(e)| + |N_v^{G(U)}(e)||N_u^{G}(e)|\right),$$

$$Sz^{**}(G(U)) = \frac{1}{2}\sum_{e=uv \in E(G(U))} \left(|N_u^{G(U)}(e)||N_u^{G}(e)| + |N_v^{G(U)}(e)||N_v^{G}(e)|\right).$$

Therefore, it is clear that if $U = V(G)$, then $Sz^{**}(G) = Sz(G)$.

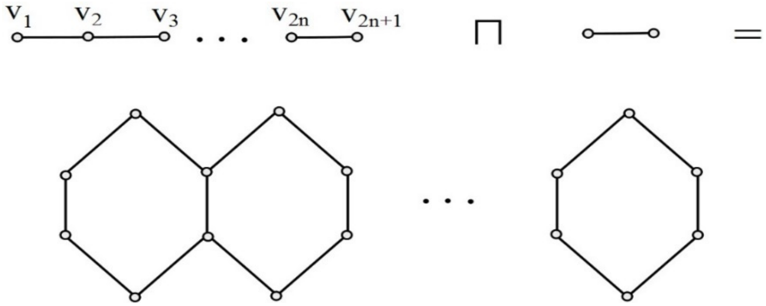

Figure 1. Hexagonal chain $L_n = P_{2n+1}(U) \sqcap P_2$, where $U = \{v_1, v_3, v_5, \ldots, v_{2n+1}\}$.

Lemma 1. (See [12]). Let G and H be graphs with $U \subseteq V(G)$. Then we have

(a) If $U = V(G)$, then the generalized hierarchical product $G(U) \sqcap H$ is the Cartesian product of G and H,
(b) $|V(G(U) \sqcap H)| = |V(G)||V(H)|$, $|E(G(U) \sqcap H)| = |E(G)||V(H)| + |E(H)||U|$,
(c) $G(U) \sqcap H$ is connected if and only if G and H are connected,

(d) $d_{G(U)\Pi H}((g,h),(g',h')) = \begin{cases} d_{G(U)}(g,g') + d_H(h,h') & \text{if } h \neq h', \\ d_G(g,g') & \text{if } h = h'. \end{cases}$

Theorem 2. Let *G* and *H* be two connected graphs and let *U* be a nonempty subset of *V(G).* Then

$$Sz^*(G(U)\Pi H) = |V(H)|(|V(H)|-1)^2 Sz^*(G(U)) + |V(H)|Sz^*(G) + |V(H)|(|V(H)|-1)\left(Sz^{**}(G(U)) - Sz^{***}(G(U))\right) + \frac{1}{2}|E(G)||V(G)|^2|V(H)|(|V(H)|-1) + |U||V(G)|^2 Sz^*(H).$$

Proof. Let *G* and *H* be two connected graphs and let *U* be a nonempty subset of *V(G).* For our convenience, we partition the edge set of $G(U)\ \Pi H$ into two sets,

$$E_1 = \{(g,h)(g',h') \mid gg' \in E(G) \text{ and } h = h' \in V(H)\},$$
$$E_2 = \{(g,h)(g',h') \mid hh' \in E(H) \text{ and } g = g' \in U\}.$$

Let $e = (g,h)(g',h) \in E_1$. Suppose $(x,y) \in V(G(U)\ \Pi H)$, thus by Lemma 1, $(x,y) \in N^{G(U)\Pi H}_{(g,h)}(e)$, if $y = h$ and $x \in N^G_g(gg')$ or, $y \neq h$ and $x \in N^{G(U)}_g(gg')$. Therefore, we have

$$|N^{G(U)\Pi H}_{(g,h)}(e)| = (|V(H)|-1)\,|N^{G(U)}_g(gg')| + |N^G_g(gg')|,$$
$$|N^{G(U)\Pi H}_{(g',h)}(e)| = (|V(H)|-1)\,|N^{G(U)}_{g'}(gg')| + |N^G_{g'}(gg')|,$$
$$|N^{G(U)\Pi H}_0(e)| = (|V(H)|-1)\,|N^{G(U)}_0(gg')| + |N^G_0(gg')|.$$

Thus, the summation of $[|N^{G(U)\Pi H}_{(g,h)}(e)| + \frac{1}{2}|N^{G(U)\Pi H}_0(e)|] \times [|N^{G(U)\Pi H}_{(g',h')}(e)| + \frac{1}{2}|N^{G(U)\Pi H}_0(e)|]$ over all edges of E_1, is equal to:

$$Sz_1 = |V(H)|(|V(H)|-1)^2 Sz^*(G(U)) + |V(H)|Sz^*(G) + |V(H)|(|V(H)|-1)\left(Sz^{**}(G(U)) - Sz^{***}(G(U))\right) + \frac{1}{2}|E(G)||V(G)|^2|V(H)|(|V(H)|-1).$$

On the other hand, assume that $e = (g,h)(g,h') \in E_2$ and let $(x,y) \in V(G(U)\ \Pi H)$, thus by Lemma 1, $(x,y) \in N^{G(U)\Pi H}_{(g,h)}(e)$ if $y \in N^H_h(hh')$. Then

$$|N^{G(U)\Pi H}_{(g,h)}(e)| = |V(G)||\,N^H_h(hh')|, \quad |N^{G(U)\Pi H}_{(g,h')}(e)| = |V(G)||\,N^H_{h'}(hh')|,$$

$$|N_0^{H(U)\Pi H}(e)| = |V(G)||N_0^{H}(hh')|.$$

Therefore, the summation of

$$[|N_{(g,h)}^{G(U)\Pi H}(e)| + \tfrac{1}{2}|N_0^{G(U)\Pi H}(e)|][|N_{(g',h')}^{G(U)\Pi H}(e)| + \tfrac{1}{2}|N_0^{G(U)\Pi H}(e)|]$$

over all edges of E_2, is equal to:

$$Sz_2 = |U||V(G)|^2 Sz^*(H).$$

By summation of Sz_1 and Sz_2, the result can be proved. □

By definition of Sz^*, Sz^{**} and Sz^{***}, we have

$$2Sz^*(G) - Sz^{**}(G) + Sz^{***}(G) = \frac{1}{2}|E(G)||V(G)|^2.$$

In the above theorem, if we set $U = V(G)$, then by the above equality, we obtain the following corollary.

Corollary 3. Let G and H be two connected graphs. Then

$$Sz^*(G\times H) = |V(H)|^3 Sz^*(G) + |V(G)|^3 Sz^*(H).$$ □

Theorem 4. Let G and H be two connected graphs and let U be a nonempty subset of $V(G)$. Then

$$M_1^*(G(U)\,\Pi H) = |V(H)|M_1^*(G(U)) + |U|M_1^*(H) + 2|E(G)|\zeta(H) + 2|E(H)|\sum_{u\in U}\varepsilon_{G(U)}(u).$$

Proof. Let G and H be two connected graphs and let U be a nonempty subset of $V(G)$. For our convenience, we partition the edge set of $G(U)\,\Pi H$ into two sets,

$$E_1 = \{(g,h)(g',h') \mid gg' \in E(G) \text{ and } h = h' \in V(H)\},$$

$$E_2 = \{(g,h)(g',h') \mid hh' \in E(H) \text{ and } g = g' \in U\}.$$

Suppose $(x,y) \in V(G(U)\,\Pi H)$, then by Lemma 1,

$$\varepsilon_{G(U)\Pi H}((x,y)) = \varepsilon_{G(U)}(x) + \varepsilon_H(y).$$

Therefore,

$$M_1^*(G(U)\Pi H) = \sum_{(g,h)(g',h')\in E(G(U)\Pi H)}[\varepsilon_{G(U)\Pi H}((g,h)) + \varepsilon_{G(U)\Pi H}((g',h'))]$$

$$= \sum_{(g,h)(g',h)\in E_1} [\varepsilon_{G(U)\Pi H}((g,h)) + \varepsilon_{G(U)\Pi H}((g',h))]$$

$$+ \sum_{(g,h)(g,h')\in E_2} [\varepsilon_{G(U)\Pi H}((g,h)) + \varepsilon_{G(U)\Pi H}((g,h'))]$$

$$= \sum_{h\in V(H)} \sum_{gg'\in E(G)} \left(\varepsilon_{G(U)}(g) + 2\varepsilon_H(h) + \varepsilon_{G(U)}(g')\right)$$

$$+ \sum_{g\in U} \sum_{hh'\in E(H)} \left(2\varepsilon_{G(U)}(g) + \varepsilon_H(h) + \varepsilon_H(h')\right) = |V(H)|M_1^*(G(U))$$

$$+ |U|M_1^*(H) + 2|E(G)|\zeta(H) + 2|E(H)| \sum_{u\in U} \varepsilon_{G(U)}(u). \qquad \square$$

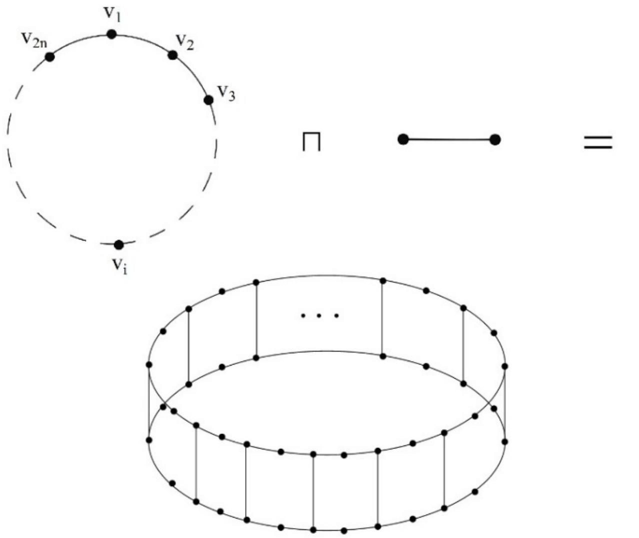

Figure 2. The zig-zag polyhex nanotube $TUHC_6[2n,2] = C_{2n}(U)\ \Pi\ P_2$, where $U = \{v_2, v_4, \ldots, v_{2n}\}$.

By a similar argument as in the proof of the previous theorem, we have:

Theorem 5. Let G and H be two connected graphs and let U be a nonempty subset of $V(G)$. Then

i). $M_2^*(G(U)\ \Pi\ H) = |V(H)|M_2^*(G(U)) + |U|M_2^*(H) + \zeta(H)M_1^*(G(U)) + |E(G)|M_1^{**}(H) + |E(H)| \sum_{u\in U} (\varepsilon_{G(U)}(u))^2 + M_1^*(H) \sum_{u\in U} \varepsilon_{G(U)}(u).$

ii). $M_1^{**}(G(U)\ \Pi\ H) = |V(H)|M_1^{**}(G(U)) + |V(G)|M_1^{**}(H) + 2\zeta(G(U))\zeta(H).$ $\square$

The exact formulas for M_2^* of the Cartesian product of graphs were obtained in [9]. We claim that this result is incorrect. The aim of the next corollary is to improve this result. In the part (*i*) of the above theorem, if we set $U = V(G)$, we obtain the following corollary.

Corollary 6. Let *G* and *H* be two connected graphs. Then

$$M_2^*(G \times H) = |V(H)|M_2^*(G) + |E(G)|M_1^{**}(H) + \zeta(H)M_1^*(G) + |V(G)|M_2^*(H) + |E(H)|M_1^{**}(G) + \zeta(G)M_1^*(H). \qquad \square$$

For the graphs in Figs.1 and 2, namely, zig-zag polyhex nanotube $TUHC_6[2n,2]$ and hexagonal chain L_n , some graph invariants were studied in [15, 16, 17, 18]. Here we obtain Sz^*, M_1^*, M_2^* and M_1^{**} of zig-zag polyhex nanotube and the hexagonal chain L_n.

Example 7. Consider the zig-zag polyhex nanotube $TUHC_6[2n,2]$ (see Fig. 2). Diudea, who was the first chemist which considered the problem of computing topological indices of nanostructures, introduced the notation $TUHC_6$. The zig-zag polyhex nanotube is the graph $C_{2n}(U)\,\Pi\, P_2$, where $U = \{v_2, v_4, \ldots, v_{2n}\}$, see Fig. 2. On the other hand, one can easily see that $Sz^{**}(C_{2n}(U)) = Sz^{***}(C_{2n}(U)) = Sz^*(C_{2n}) = 2n^3$ and $Sz^*(C_{2n}(U)) = 2n(n^2 - 1)$ and so, by Theorem 2, we have

$$Sz^*(TUHC_6[2n,2]) = 20n^3 - 4n.$$

Example 8. Consider the hexagonal chain L_n (see Fig. 1). The hexagonal chain L_n is the graph $P_{2n+1}(U)\,\Pi\, P_2$, where $U = \{v_1, v_3, \ldots, v_{2n+1}\}$, see Fig. 1. On the other hand, it is not difficult to check that $Sz^*(P_{2n+1}) = Sz^*(P_{2n+1}(U)) = \frac{4}{3}n^3 + 2n^2 + \frac{2}{3}n$, $Sz^{**}(P_{2n+1}(U)) = \frac{4}{3}n^3 + 2n^2 + \frac{5}{3}n$ and $Sz^{***}(P_{2n+1}(U)) = \frac{8}{3}n^3 + 2n^2 - \frac{2}{3}n$ and so, by Theorem 2, we obtain

$$Sz^*(L_n) = \frac{44}{3}n^3 + 24n^2 + \frac{43}{3}n + 1.$$

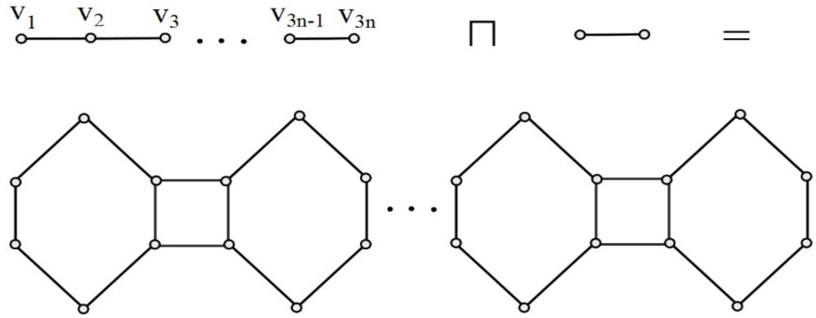

Figure 3. The linear phenylene $F_n = P_{3n}(U) \sqcap P_2$, where
$U = \{v_{3k+1} \mid 0 \leq k \leq n-1\} \cup \{v_{3k} \mid 1 \leq k \leq n\}$.

Example 9. Consider the linear phenylene F_n including n benzene ring (see Fig. 3). The linear phenylene F_n is the graph $P_{3n}(U) \sqcap P_2$, where $U = \{v_{3k+1} \mid 0 \leq k \leq n-1\} \cup \{v_{3k} \mid 1 \leq k \leq n\}$, see Fig. 3. On the other hand, it is not difficult to check that $Sz^*(P_{3n}) = Sz^*(P_{3n}(U)) = \frac{9}{2}n^3 - \frac{1}{2}n$, $Sz^{**}(P_{3n}(U)) = \frac{9}{2}n^3 + \frac{1}{2}n$ and $Sz^{***}(P_{3n}(U)) = 9n^3 - \frac{9}{2}n^2 - \frac{1}{2}n$ and so, by Theorem 2, we obtain $Sz^*(F_n) = Sz^*(P_{3n}(U) \sqcap P_2) = 54n^3$.

In [19, Example 3.2], the authors claim that $Sz(F_n) = 54n^3 - 4n$. We claim that this result is incorrect. By [19, Example 3.2], $Sz(F_1) = 50$ and $Sz(F_2) = 424$ that, are incorrect. The correct values are $Sz(F_1) = 54$ and $Sz(F_2) = 432$. Note that F_n is bipartite and so $Sz^*(F_n) = Sz(F_n)$. On the other hand, by the above example, $Sz^*(F_n) = 54n^3$ and so, $Sz(F_n) = 54n^3$.

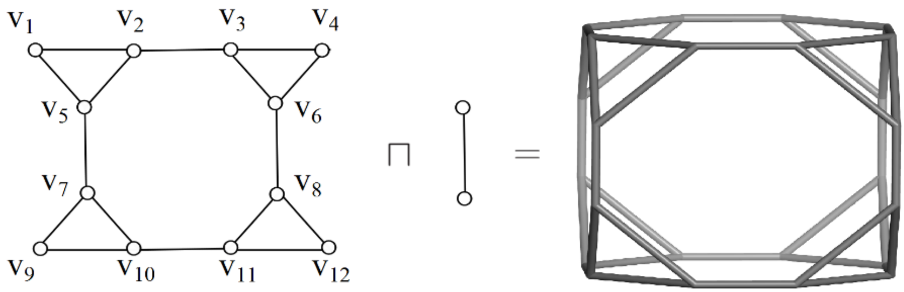

Figure 4. The molecular graph of truncated cube $H = G(U) \sqcap P_2$,
where $U = \{v_1, v_4, v_9, v_{12}\}$.

Example 10. Let H be the graph of truncated cube. Then $H = G(U)\ \Pi\ P_2$, where $U = \{v_1, v_4, v_9, v_{12}\}$, as shown in Figure 4. It is not difficult to check that $Sz^*(G) = Sz^*(G(U)) = 526$, $Sz^{**}(G(U)) = 380$, $Sz^{***}(G(U)) = 280$ and so, by Theorem 2, we have $Sz^*(H) = Sz^*(G(U)\ \Pi\ P_2) = 3264$.

Example 11. Consider the hexagonal chain L_n and the zig-zag polyhex nanotube $TUHC_6[2n,2]$ *and truncated cube* H depicted in Figs. 1, 2 and 4, respectively, such that n > 1. One can easily see that $M_1^*(P_{2n+1}(U)) = 6n^2$, $M_2^*(P_{2n+1}(U)) = \frac{14}{3}n^3 - \frac{2}{3}n$, $M_1^*(C_{2n}(U)) = 4n^2$, $M_2^*(C_{2n}(U)) = M_1^{**}(C_{2n}(U)) = M_1^{**}(C_{2n}) = 2n^3$, $M_1^*(G(U)) = 160$, $M_2^*(G(U)) = 400$, $\sum_{g\in U}\varepsilon_{C_{2n}(U)}(g) = n^2$,

$$\sum_{g\in U}(\varepsilon_{C_{2n}(U)}(g))^2 = n^3,\quad \sum_{g\in U}\varepsilon_{P_{2n+1}(U)}(g) = \begin{cases}\frac{3}{2}n^2 + 2n + \frac{1}{2} & 2 / n\\ \frac{3}{2}n^2 + 2n & 2 / n\end{cases},$$

$$\sum_{g\in U}(\varepsilon_{P_{2n+1}(U)}(g))^2 = \begin{cases}\frac{7}{3}n^3 + 4n^2 + \frac{5}{3}n & 2 / n\\ \frac{7}{3}n^3 + 4n^2 + \frac{2}{3}n & 2 / n\end{cases},\quad \sum_{g\in U}\varepsilon_{G(U)}(g) = 20,$$

$\sum_{g\in U}(\varepsilon_{G(U)}(g))^2 = 10$ and so, by Theorems 4 and 5, for n > 1, we have:

1. $M_1^*(L_n) = M_1^*(P_{2n+1}(U)\ \Pi\ P_2) = \begin{cases}15n^2 + 14n + 3 & 2 / n\\ 15n^2 + 14n + 2 & 2 / n\end{cases}$.
2. $M_1^*(TUHC_6[2n,2]) = M_1^*(C_{2n}(U)\ \Pi\ P_2) = 10n(n+1)$.
3. $M_2^*(L_n) = M_2^*(P_{2n+1}(U)\ \Pi\ P_2) = \begin{cases}\frac{35}{3}n^3 + 19n^2 + \frac{28}{3}n + 2 & 2 / n\\ \frac{35}{3}n^3 + 19n^2 + \frac{25}{3}n + 1 & 2 / n\end{cases}$.
4. $M_2^*(TUHC_6[2n,2]) = M_2^*(C_{2n}(U)\ \Pi\ P_2) = 5n^3 + 10n^2 + 5n$.
5. $M_1^*(H) = M_1^*(G(U)\ \Pi\ P2) = 432$.
6. $M_2^*(H) = M_2^*(G(U)\ \Pi\ P_2) = 1296$.

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