Research Article

Comparative Study of Generalized Sum Graphs via Degree-Based Topological Indices

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In theoretical chemistry, topological indices (TIs) have important role to predict various physical and structural properties of the study under molecular graphs. Among all topological indices, Zagreb-type indices have been used more effectively in the chemical literature. In this paper, we have computed first Zagreb, second Zagreb, forgotten, and hyper Zagreb indices of the generalized Q-sum graph $(H_{1(Q_\alpha)}[H_2])$ in the form of different TIs of its basic graphs, where $\alpha \geq 1$ is a positive integer. This family of graphs is obtained by the lexicographic product of the graph $Q_\alpha(H_1)$ and H_2 , where $Q_\alpha(H_1)$ is constructed with the help of the generalized line superposition operation Q_α on H_1 . As a conclusion, we also checked the correlation between predefined graph $H_1[H_2]$ under the operation of lexicographic product H_1 and H_2 with newly defined generalized Q-sum graphs $(H_{1(Q_\alpha)}[H_2])$ using linear regression models of various degree-based TIs.

1. Introduction and Preliminaries

In the computing analysis of chemical compounds, the chemical structural formulas are usually represented by graphs. Mathematically, for a graph H , the vertex and edge sets are denoted by $V(H)$ and $E(H) \subseteq V(H) \times V(H)$, respectively. The degree of the vertex $z \in V(H)$ (denoted by $d(z)$) is the number of incident edges on it. The distance between any two vertices z and y in $V(H)$ is denoted by $d(z, y)$ and defined as the number of edges in a shortest path existing between the vertices z and y . Thoroughly, the graph H is considered as a finite and simple graph.

The subject of chemical graph theory has many applications in chemistry. In a chemical graph, a vertex and an edge correspond to an atom and a chemical bond between them, respectively. A topological index is a function which presents a chemical graph in the form of a numerical number that is used to model the chemical and physical properties of molecules in quantitative structure property and activity relationships.

For a molecular graph H , the first Zagreb index $M_1(H)$ and second Zagreb index $M_2(H)$ are firstly considered by Gutman and Trinajstić [1] in 1972 to study the total π electron energy of the molecular graph H which are defined as follows:

$$\begin{aligned} M_1(H) &= \sum_{z \in V(H)} d^2(z) = \sum_{zy \in E(H)} [d(z) + d(y)], \\ M_2(H) &= \sum_{zy \in E(H)} [d(z) \times d(y)]. \end{aligned} \quad (1)$$

In 2015, forgotten index (F index) is defined as follows [2]:

$$F(H) = \sum_{z \in V(H)} d^3(z) = \sum_{zy \in E(H)} [d^2(z) + d^2(y)]. \quad (2)$$

In 2005, the first general Zagreb index is defined as follows [3]:

$$M_1^{\beta+1}(H) = \sum_{z \in V(H)} d^{\beta+1}(z) = \sum_{zy \in E(H)} [d^{\beta}(z) + d^{\beta}(y)]. \quad (3)$$

The concept of the general randic index (GRI) is defined by Bollobas and Erdos as

$$R_{\beta}(H) = \sum_{zy \in E(H)} [d(z) \times d(y)]^{\beta}. \quad (4)$$

In 2013, hyper Zagreb index is defined by Shirdel et al. as follows [4]:

$$HM(H) = \sum_{zy \in E(H)} [d(z) + d(y)]^2. \quad (5)$$

For more studies, we refer to [5]. In particular, we can find the results of TIs for various families of graphs such as nanosheets & nanostars dendrimers [6, 7], hex-derived networks [8], benzene networks [9, 10], and cellulose networks [11]. In addition, for the studies of the complex graphs, operations on graphs play a key role, where the original graphs are called the factors of the newly constructed graph under operations [12].

Yan et al. [13] defined the line superposition operation Q_1 related to the subdivision of H and computed the Wiener index of this derived graph $Q_1(H)$, where $Q_1(H)$ is obtained by inserting one new vertex in every edge of H and joining those pairs of new vertices by edges which have common adjacent (original) vertices (see Figure 1). Liu et al. extended this operation for any integral value of $\alpha \geq 1$ and obtained the generalized line superposition graph $Q_{\alpha}(H)$ from the graph H by inserting α vertices in each edge and joining those pairs of new vertices by edges which have common adjacent (original) vertices [14] (see Figures 2 and 3).

Taeri et al. [15] constructed the Q_1 -sum graph by Cartesian product of $Q_1(H_1)$ and H_2 , where $Q_1(H_1)$ is a line superposition graph, and H_1 and H_2 are assumed to be two connected graphs. Also, they computed the Wiener index of Q_1 -sum graph. Whereas, Chu et al. [16], Deng et al. [17], Akhter et al. [18], and Liu et al. [14] calculated the different indices of Q_1 -sum graph $(H_{1(Q_1)} + H_2)$ based on the Cartesian product. Recently, Liu et al. [19] extended this operation for any integral value of k and obtained the generalized line superposition graph $Q_k(H_1)$ of the graph H_1 . Moreover, they constructed the generalized Q -sum graph $(H_{1(Q_k)} + H_2)$ and computed their Zagreb indices. Javaid et al. [20] constructed the generalized Q -sum graph based on strong product and computed its first and second Zagreb indices.

The composition or lexicographic product of two connected graphs H_1 and H_2 , which is denoted by $H_1[H_2]$, is a graph such that the set of vertices is $V(H_1) \times V(H_2)$, and two vertices (z_1, y_1) and (z_2, y_2) will be adjacent in $H_1[H_2]$ if $[z_1 = z_2, \text{ and } y_1 \text{ is adjacent to } y_2]$ or $[z_1 \text{ is adjacent to } z_2, \text{ and } y_1 \text{ is adjacent to } y_2]$.

Sarala et al. [21], De [22], Pattabiraman [23], Pattabiraman and Santhakumar [24], and Suresh and Devi [25] have computed different degree-related Zagreb indices for the graphs based on line superposition operation and lexicographic product.

FIGURE 1: Line superposition operation for P_3 denoted by $Q_1(P_3)$.

FIGURE 2: Generalized line superposition operation for P_3 and $\alpha = 2$ denoted by $Q_2(P_3)$.

FIGURE 3: Generalized line superposition operation for P_3 for $\alpha = 3$ denoted by $Q_3(P_3)$.

(1) Q_{α} -sum: let H_1 and H_2 be two graphs; first, we apply generalized line superposition operation on H_1 to get $Q_{\alpha}(H_1)$ graph. Then, we take lexicographic product between $Q_{\alpha}(H_1)$ and H_2 to get Q_{α} -Sum graph denoted by $H_{1(Q_{\alpha})}[H_2]$. Q_{α} -sum graph having vertex-set

$$\begin{aligned} V(H_{1(Q_{\alpha})}[H_2]) &= V(Q_{\alpha}(H_1)) \times V(H_2) \\ &= (V(H_1) \cup \alpha(E(H_1))) \times V(H_2), \end{aligned} \quad (6)$$

such that two vertices (z_1, y_1) and (z_2, y_2) of $V(H_{1(Q_{\alpha})}[H_2])$ are adjacent if $[z_1 = z_2 \text{ in } V(H_1), \text{ and } y_1 \text{ is adjacent to } y_2 \text{ in } E(H_2)]$ or $[z_1 \text{ is adjacent to } z_2 \text{ in } E(Q_{\alpha}(H_1)), \text{ and } y_1 \text{ is adjacent to } y_2 \text{ in } E(H_2)]$, where $\alpha \geq 1$ is a positive integer (see Figure 4).

To check the correlation between the predefined lexicographic product of two simple graphs $(H_1[H_2])$ and newly defined Q_{α} -sum graphs $(H_{1(Q_{\alpha})}[H_2])$, one may use the linear regression when having a linear relationship between the dependent variable ($X = H_1[H_2]$) and the independent variable ($Y = H_{1(Q_{\alpha})}[H_2]$). For further studies related to operations and graph products, the readers are referred to

FIGURE 4: Generalized Q_α -sum graph $H_{1(Q_\alpha)}[H_2]$ for $P_{3(Q_3)}[P_2]$.

[26–29]. In this paper, we have used the generalized line superposition operation to construct a new generalized line

superposition graph $Q_\alpha(H_1)$ from the graph actual graph H_1 . Then, we have constructed a Q_α -sum graph based on the lexicographic product of $Q_\alpha(H_1)$ and H_2 , denoted by $H_{1(Q_\alpha)}[H_2]$. Moreover, we have computed the first Zagreb, second Zagreb, forgotten, and hyper Zagreb indices of $H_{1(Q_\alpha)}[H_2]$ in terms of its factor graphs H_1 and H_2 . We have extended this work by constructing linear regression models between $(H_1[H_2])$ and Q_α -sum graphs $(H_{1(Q_\alpha)}[H_2])$ via foresaid degree-based TIs.

2. Main Results

This section covers the main results.

Theorem 1. Let H_1 and H_2 be two connected graphs such that $|V(H_1)|, |V(H_2)| \geq 4$. For $\alpha \geq 1$,

$$M_1(H_{1(Q_\alpha)}[H_2]) = 8|V(H_2)||E(H_1)||E(H_2)| + 3|V(H_2)|^3 M_1(H_1) + |V(H_1)| M_1(H_2) + 2(\alpha - 1)|V(H_2)|^2 M_1(H_1) + (\alpha)|V(H_2)|^3 [M_3(H_1) + 2M_2(H_1) - 2M_1(H_1)]. \quad (7)$$

Proof.

$$\begin{aligned} M_1(H_{1(Q_\alpha)}[H_2]) &= \sum_{(z_1, y_1), (z_2, y_2) \in E(H_{1(Q_\alpha)}[H_2])} [d(z_1, y_1) + d(z_2, y_2)] \\ &= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [d(z, y_1) + d(z, y_2)] + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1, z_2 \in E(Q_\alpha(H_1))} [d(z_1, y_1) + d(z_2, y_2)] \\ &= \sum_A + \sum_B. \end{aligned} \quad (8)$$

Now,

$$\begin{aligned} \sum_A &= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [d(z, y_1) + d(z, y_2)] = \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [2|V(H_2)|d_{H_1}(z) + d_{H_2}(y_1) + d_{H_2}(y_2)] \\ &= 4|V(H_2)||E(H_1)||E(H_2)| + |V(H_1)| M_1(H_2), \\ \sum_B &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1, z_2 \in E(Q_\alpha(H_1))} [d(z_1, y_1) + d(z_2, y_2)] \end{aligned}$$

$$\begin{aligned}
&= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1) + d(z_2, y_2)] + \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y) + d(z_2, y)] \\
&+ \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1) + d(z_2, y_1)] = \sum_{B_1} + \sum_{B_2} + \sum_{B_3}, \\
\sum_{B_1} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1) + d(z_2, y_2)] \\
&= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_1) + d_{H_2}(y_1) + |V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right] \\
&= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_2)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{H_1}(z_1) + d_{H_2}(y_1) \right] \\
&+ \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_2)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right] \\
&= 4|V(H_2)| \|E(H_1)\| E(H_2) + |V(H_2)|^3 M_1(H_1) \\
&+ \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right]. \tag{9}
\end{aligned}$$

For $z_2 \in V(Q_\alpha(H_1)) - V(H_1)$ which is inserted into the edge uv of (H_1) , we have $d_{Q_\alpha(H_1)}(z_2) = d_{H_1}(u) + d_{H_1}(v)$. This gives

$$\begin{aligned}
&\sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[d_{Q_\alpha(H_1)}(z_2) \right] = 2 \sum_{uv \in E(H_1)} [d_{H_1}(u) + d_{H_1}(v)] = 2M_1(H_1) \\
&\sum_{H_2} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[d_{Q_\alpha(H_1)}(z_2) \right] = 2|V(H_2)| M_1(H_1). \tag{10}
\end{aligned}$$

So, we have

$$\sum_{B_1} = 4|V(H_2)| \|E(H_1)\| E(H_2) + 3|V(H_2)|^3 M_1(H_1). \tag{11}$$

Now, we take

$$\sum_{B_2} = \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y) + d(z_2, y)]$$

$$\begin{aligned}
&= \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_1) + |V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right] \\
&= 2(\alpha - 1) |V(H_2)|^2 \sum_{uv \in E(H_1)} [d_{H_1}(u) + d_{H_1}(v)] = 2(\alpha - 1) |V(H_2)|^2 M_1(H_1), \\
\sum_{B_3} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_1) + |V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right] \\
&= |V(H_2)|^3 (\alpha) \sum_{\substack{uv \in E(H_1) \\ vw \in E(H_2)}} [d_{H_1}(u) + d_{H_1}(v) + d_{H_1}(v) + d_{H_1}(w)], \tag{12}
\end{aligned}$$

where z_1 and z_2 are the vertices that are inserted into the edges uv of H_1 and vw of H_1 , respectively.

$$\begin{aligned}
&= (\alpha) |V(H_2)|^3 \left[\sum_{v \in V(H_1)} d_{H_1}^3(v) - d_{H_1}^2(v) + \sum_{v \in V(H_1)} (d_{H_1}(v) - 1) \sum_{\substack{u \in V(H_1) \\ uv \in E(H_1)}} d_{H_1}(u) \right] \\
&= (\alpha) |V(H_2)|^3 [M_3(H_1) + 2M_2(H_1) - 2M_1(H_1)]. \tag{13}
\end{aligned}$$

Consequently, we have obtained our required result. $\square$

Theorem 2. Let H_1 and H_2 be two connected graphs such that $|V(H_1)|, |V(H_2)| \geq 4$. For $\alpha \geq 1$,

$$\begin{aligned}
M_2(H_{1(Q_\alpha)}[H_2]) &= 5|E(H_2)| |V(H_2)|^2 M_1(H_1) + 2|E(H_1)| |V(H_2)| M_1(H_2) + |V(H_1)| M_2(H_2) \\
&\quad + |V(H_2)|^4 [M_3(H_1) + 2M_2(H_1)] + (\alpha) |V(H_2)|^4 \\
&\quad \left[\frac{1}{2} M_4(H_1) - \frac{1}{2} M_3(H_1) + \sum_{uv \in V(H_1)} r d(u) d(v) \right] \\
&\quad + \sum_{v \in V(H_1)} d^2(v) \sum_{\substack{u \in V(H_1) \\ uv \in E(H_1)}} d(u) - 2M_2(H_1) + (\alpha - 1) |V(H_2)|^3 [2M_2(H_1) + M_3(H_1)], \tag{14}
\end{aligned}$$

where r is the number of neighbours which are common between u and v in H_1 . *Proof.*

$$\begin{aligned}
 M_2(H_1(Q_\alpha)[H_2]) &= \sum_{(z_1, y_1)(z_2, y_2) \in E(H_1(Q_\alpha)[H_2])} [d(z_1, y_1)d(z_2, y_2)] \\
 &= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [d(z, y_1)d(z, y_2)] + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1, z_2 \in E(Q_\alpha(H_1))} [d(z_1, y_1)d(z_2, y_2)] \\
 &= \sum_A + \sum_B.
 \end{aligned} \tag{15}$$

Now, we take

$$\begin{aligned}
 \sum_A &= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [d(z, y_1)d(z, y_2)] \\
 &= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [|V(H_2)|d_{H_1}(z) + d_{H_2}(y_1)][|V(H_2)|d_{H_1}(z) + d_{H_2}(y_2)] \\
 &= |E(H_2)||V(H_2)|^2 M_1(H_1) + 2|E(H_1)||V(H_2)|M_1(H_2) + |V(H_1)|M_2(H_2), \\
 \sum_B &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1, z_2 \in E(Q_\alpha(H_1))} [d(z_1, y_1)d(z_2, y_2)] \\
 &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_2)}} [d(z_1, y_1)d(z_2, y_2)] \sum_{y \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1, z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y)d(z_2, y)] \\
 &\quad + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1, z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1)d(z_2, y_2)] = \sum_{B_1} + \sum_{B_2} + \sum_{B_3}.
 \end{aligned} \tag{16}$$

So,

$$\begin{aligned}
 \sum_{B_1} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1)d(z_2, y_2)] \\
 &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [|V(H_2)||d_{H_1}(z_1) + d_{H_2}(y_1)][|V(H_2)|d_{Q_\alpha(H_1)}(z_2)] \\
 &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [|V(H_2)|d_{Q_\alpha(H_1)}(z_2)d_{H_2}(y_1) + |V(H_2)|^2 d_{H_1}(z_1)d_{Q_\alpha(H_1)}(z_2)]
 \end{aligned}$$

$$\begin{aligned}
&= |V(H_2)|^4 \sum_{\substack{z_1 z_2 \in E(Q(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q(H_1)) - V(H_1)}} d_{Q_\alpha(H_1)}(z_1) d_{Q_\alpha(H_1)}(z_2) + 2|E(H_2)|^2 \sum_{\substack{z_1 z_2 \in E(Q(H_1)) \\ z_1 \in V(H_1) \\ z_2 \in V(Q(H_1)) - V(H_1)}} d_{Q_\alpha(H_1)}(z_2) \\
&= |V(H_2)|^4 \sum_{\substack{z_1 z_2 \in E(Q(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q(H_1)) - V(H_1)}} d_{Q_\alpha(H_1)}(z_1) d_{Q_\alpha(H_1)}(z_2) + 4|E(H_2)|^2 M_1(H_1), \tag{17}
\end{aligned}$$

where z_2 is the vertex inserted into the edge $z_1 w_1$ of H_1

$$\begin{aligned}
&= |V(H_2)|^4 \sum_{z_1 \in V(H_1)} \sum_{w_1 \in V(N_{H_1}(z_1))} d_{Q_\alpha(H_1)}(z_1) [d_{Q_\alpha(H_1)}(z_1) + d_{Q_\alpha(H_1)}(w_1)] \\
&\quad + 4|E(H_2)|^2 M_1(H_1), \tag{18}
\end{aligned}$$

where $N_{H_1}(z_1)$ is the set of neighbor vertices of z_1 in H_1

$$\begin{aligned}
&= |V(H_2)|^4 [M_3(H_1) + 2M_2(H_1)] + 4|E(H_2)|^2 M_1(H_1), \\
\sum_{B_2} &= \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y) d(z_2, y)] \\
\sum_{B_2} &= \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [|V(H_2)| d_{Q_\alpha(H_1)}(z_1)] [|V(H_2)| d_{Q_\alpha(H_1)}(z_2)] \\
&= (\alpha - 1) |V(H_2)|^3 [2M_2(H_1) + M_3(H_1)], \tag{19} \\
\sum_{B_3} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [|V(H_2)| d_{Q_\alpha(H_1)}(z_1)] [|V(H_2)| d_{Q_\alpha(H_1)}(z_2)] \\
&= |V(H_2)|^2 (\alpha) \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{uv \in E(H_1) \\ vw \in E(H_2)}} [d_{H_1}(u) + d_{H_1}(v)] [d_{H_1}(v) + d_{H_1}(w)],
\end{aligned}$$

where z_1 is the added vertex in the edge uv , and z_2 is the added vertex in the edges vw of H_1

$$\begin{aligned}
&= (\alpha) |V(H_2)|^4 \left[\frac{1}{2} \sum_{v \in V(H_1)} (d_{H_1}^4(v) - d_{H_1}^3(v)) + \sum_{uv \in V(H_1)} r d_{H_1}(u) d_{H_1}(v) + \sum_{v \in V(H_1)} d_{H_1}^2(v) \right. \\
&\quad \left. \times \sum_{\substack{u \in V(H_1) \\ uv \in E(H_1)}} d_{H_1}(u) - 2M_2(H_1) \right] \\
&= (\alpha) |V(H_2)|^4 \left[\frac{1}{2} M_4(H_1) - \frac{1}{2} M_3(H_1) + \sum_{uv \in V(H_1)} r d_{H_1}(u) d_{H_1}(v) \right. \\
&\quad \left. + \sum_{v \in V(H_1)} d_{H_1}^2(v) \sum_{\substack{u \in V(H_1) \\ uv \in E(H_1)}} d_{H_1}(u) - 2M_2(H_1) \right].
\end{aligned} \tag{20}$$

where r is the number of neighbors which are common vertices of u and v in (H_1) . Consequently, we have obtained our required result. $\square$

Theorem 3. Let H_1 and H_2 be two connected graphs such that $|V(H_1)|, |V(H_2)| \geq 4$. For $\alpha \geq 1$,

$$\begin{aligned}
F(H_{1(Q_\alpha)}[H_2]) &= 3|V(H_2)|^4 F(H_1) + |V(H_1)| F(H_2) + 6|V(H_2)|^2 |E(H_2)| M_1(H_1) + 6|V(H_2)| \\
&\quad \times |E(H_1)| M_1(H_2) + 4|V(H_2)|^4 M_2(H_1) + (\alpha) |V(H_2)|^4 [M_4(H_1) - F(H_1) - 4M_2(H_1) \\
&\quad + \sum_{u \in V(H_1)} \left(\sum_{v \in N_{H_1}(u)} d_{H_1}(u) (d_{H_1}(v) - 1) \right) + \sum_{uv \in E(H_1)} d_{H_1}(u) d_{H_1}(v) (d_{H_1}(u) \\
&\quad + d_{H_1}(v))] + 2(\alpha - 1) |V(H_2)|^3 F(H_1).
\end{aligned} \tag{21}$$

Proof.

Consider

$$\begin{aligned}
F(H_{1(Q_\alpha)}[H_2]) &= \sum_{(z_1, y_1), (z_2, y_2) \in E(H_{1(Q_\alpha)}[H_2])} [d(z_1, y_1)^2 + d(z_2, y_2)^2] \\
&= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [d(z, y_1)^2 + d(z, y_2)^2] + \sum_{y \in V(H_2)} \sum_{z_1, z_2 \in E(Q_\alpha(H_2))} [d(z_1, y)^2 + d(z_2, y)^2] \\
&= \sum_A + \sum_B.
\end{aligned} \tag{22}$$

Now,

$$\begin{aligned}
\sum_A &= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [(d_{H_1}(z) + d_{H_2}(y_1))^2 + (d_{H_1}(z) + d_{H_2}(y_2))^2] \\
&= \sum_{z \in V(H_1)} \sum_{y_1, y_2 \in E(H_2)} [2|V(H_2)|^2 d_{H_1}(z)^2 + (d_{H_2}(y_1)^2 + d_{H_2}(y_2)^2) + 2d_{H_1}(z) |V(H_1)| (d_{H_2}(y_1) + d_{H_2}(y_2))] \\
&= \sum_{z \in V(H_1)} [|E(H_2)| |V(H_2)|^2 \times 2d_{H_1}(z)^2 + F(H_2) + 2|V(H_2)| M_1(H_2) d_{H_1}(z)]
\end{aligned}$$

$$\begin{aligned}
&= 2|E(H_2)|V(H_2)^2 M_1(H_1) + |V(H_1)|F(H_2) + 4|V(H_2)|E(H_1)|M_1(H_2), \\
\sum_B &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1 z_2 \in E(Q_\alpha(H_1))} [d(z_1, y_1)^2 + d(z_2, y_2)^2] \\
&= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1)^2 + d(z_2, y_2)^2] \\
&\quad + \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y)^2 + d(z_2, y)^2] \\
&\quad + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1)^2 + d(z_2, y_2)^2] = \sum_{B_1} + \sum_{B_2} + \sum_{B_3}. \tag{23}
\end{aligned}$$

Now, we take

$$\begin{aligned}
\sum_{B_1} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[\left(|V(H_2)|d_{Q_\alpha(H_1)}(z_1) + d_{H_2}(y_1) \right)^2 + |V(H_2)|^2 d_{Q_\alpha(H_1)}(z_2)^2 \right] \\
&= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_1)^2 + d_{H_2}(y_1)^2 + 2|V(H_2)|d_{Q_\alpha(H_1)}(z_1)d_{H_2}(y_1) \right. \\
&\quad \left. + |V(H_2)|^2 d_{Q_\alpha(H_1)}(z_2)^2 \right] \\
&= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1 \in V(H_1)} \left[|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_1)^2 + d_{H_2}(y_1)^2 + 2|V(H_2)|d_{Q_\alpha(H_1)}(z_1)d_{H_2}(y_1) \right] \\
&\quad + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_2)^2 \right] \\
&= |V(H_2)|F(H_1) + 2|E(H_1)|M_1(H_2) + 4|E(H_2)|M_1(H_1) + |V(H_2)|^2 \sum_{y \in V(H_2)} \\
&\quad \times \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d_{Q_\alpha(H_1)}(z_2)^2]. \tag{24}
\end{aligned}$$

For $z_2 \in V(Q_\alpha(H_1)) - V(H_1)$ that is introduced into the edges uv of (H_1) , we have $d_{Q_\alpha(H_1)}(z_2) = d_{H_1}(u) + d_{H_1}(v)$. This gives

$$\sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d_{Q_\alpha(H_1)}(z_2)^2] = 2 \sum_{uv \in E(H_1)} [d_{H_1}(u) + d_{H_1}(v)]^2 = 2HM(H_1). \tag{25}$$

So,

$$\begin{aligned}
\sum_{B_1} &= |V(H_2)|^4 [2HM(H_1) + F(H_1)] + 2|V(H_2)||E(H_1)||M_1(H_2) + 4|V(H_2)|^2|E(H_2)||M_1(H_1), \\
\sum_{B_2} &= \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1, z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [|V(H_2)|^2 d(z_1, y)^2 + |V(H_2)|^2 d(z_2, y)^2] \\
&= \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1, z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_1)^2 + |V(H_2)|^2 d_{Q_\alpha(H_1)}(z_2)^2] \\
&= 2(\alpha - 1)|V(H_2)|^2 \sum_{y \in V(H_2)} \sum_{uv \in E(H_1)} [d_{H_1}(u)^2 + d_{H_1}(v)^2] = 2(\alpha - 1)|V(H_2)|^3 F(H_1), \\
\sum_{B_3} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1, z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_1)^2 + |V(H_2)|^2 d_{Q_\alpha(H_1)}(z_2)^2] \\
&= (\alpha)|V(H_2)|^4 \sum_{\substack{uv \in E(H_1) \\ vw \in E(H_2)}} [(d_{H_1}(u) + d_{H_1}(v))^2 + (d_{H_1}(v) + d_{H_1}(w))^2],
\end{aligned} \tag{26}$$

where z_1 and z_2 are the nodes that are introduced into the edge set of uv and vw of H_1

$$\begin{aligned}
&= (\alpha)|V(H_2)|^4 \left[\sum_{u \in V(H_1)} d_{H_1}(v)^4 - d_{H_1}(v)^3 + \sum_{v \in V(H_1)} (d_{H_1}(v) - 1) \sum_{\substack{u \in V(H_1) \\ uv \in E(H_1)}} d_{H_1}(u)^2 \right. \\
&\quad \left. + 2 \sum_{v \in V(H_1)} d_{H_1}(v)(d_{H_1}(v) - 1) \sum_{\substack{u \in V(H_1) \\ uv \in E(H_1)}} d_{H_1}(u) \right] \\
&= (\alpha)|V(H_2)|^4 [M_4(H_1) - F(H_1) - 4M_2(H_1) + \sum_{u \in V(H_1)} \left(\sum_{v \in N_{H_1}(u)} d_{H_1}(u)(d_{H_1}(v) - 1) \right) \\
&\quad + \sum_{uv \in E(H_1)} d_{H_1}(u)d_{H_1}(v)(d_{H_1}(u) + d_{H_1}(v))],
\end{aligned} \tag{27}$$

Consequently, we have obtained our required result. $\square$

Theorem 4. Let H_1 and H_2 be two connected graphs such that $|V(H_1)|, |V(H_2)| \geq 4$. For $\alpha \geq 1$,

$$\begin{aligned}
HZ(H_{1(Q_\alpha)}[H_2]) &= \alpha|V(H_2)|^4 [HZ(L(H_1)) + 8M_1(L(H_1)) + 8M_1(H_1) - 16|E(H_1)|] \\
&\quad + 4(\alpha - 1)|V(H_2)|^3 HZ(H_1) + 12|V(H_2)|^2 |E(H_2)||M_1(H_1) + |V(H_1)||HZ(H_2) \\
&\quad + 10|V(H_2)||E(H_1)||M_1(H_2) + |V(H_2)|^4 [2HZ(H_1) + 3F(H_1) + 4M_2(H_1)].
\end{aligned} \tag{28}$$

Proof.

$$\begin{aligned}
 HZ\left(H_{1(Q_\alpha)}[H_2]\right) &= \sum_{(z_1, y_1)(z_2, y_2) \in E\left(H_{1(Q_\alpha)}[H_2]\right)} [d(z_1, y_1) + d(z_2, y_2)]^2 \\
 &= \sum_{z \in V(H_1)} \sum_{y_1 y_2 \in E(H_2)} [d(z, y_1) + d(z, y_2)]^2 + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1 z_2 \in E(Q_\alpha(H_1))} [d(z_1, y_1) + d(z_2, y_2)]^2 \\
 &= \sum_A + \sum_B.
 \end{aligned} \tag{29}$$

Now,

$$\begin{aligned}
 \sum_A &= \sum_{z \in V(H_1)} \sum_{y_1 y_2 \in E(H_2)} [d(z, y_1) + d(z, y_2)]^2 \\
 &= \sum_{z \in V(H_1)} \sum_{y_1 y_2 \in E(H_2)} \left[\left(|V(H_2)| d_{Q_\alpha(H_1)}(z) + d_{H_2}(y_1) \right) + \left(|V(H_2)| d_{Q_\alpha(H_1)}(z) + d_{H_2}(y_2) \right) \right]^2 \\
 &= \sum_{z \in V(H_1)} \sum_{y_1 y_2 \in E(H_2)} \left[2|V(H_2)| d_{Q_\alpha(H_1)}(z) + d_{H_2}(y_1) + d_{H_2}(y_2) \right]^2 \\
 &= \sum_{z \in V(H_1)} \sum_{y_1 y_2 \in E(H_2)} \left[4|V(H_2)|^2 \left(d_{Q_\alpha(H_1)}(z) \right)^2 + \left(d_{H_2}(y_1) \right)^2 + \left(d_{H_2}(y_2) \right)^2 + 4|V(H_2)| d_{Q_\alpha(H_1)}(z) d_{H_2}(y_1) \right. \\
 &\quad \left. + 4|V(H_2)| d_{Q_\alpha(H_1)}(z) d_{H_2}(y_2) + 2d_{H_2}(y_1) d_{H_2}(y_2) \right] \\
 &= 4|E(H_2)| |V(H_2)|^2 M_1(H_1) + |V(H_1)| HZ(H_2) + \sum_{z \in V(H_1)} \sum_{y_1 y_2 \in E(H_2)} 4d_{H_1}(z) [d_{H_2}(y_1) + d_{H_2}(y_2)] \\
 &= 4|E(H_2)| |V(H_2)|^2 M_1(H_1) + |V(H_1)| HZ(H_2) + 8|E(H_1)| |V(H_2)| M_1(H_2), \\
 \sum_B &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{z_1 z_2 \in E(Q_\alpha(H_1))} [d(z_1, y) + d(z_2, y)]^2 \\
 &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1) z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1) + d(z_2, y_2)]^2 \\
 &\quad + \sum_{y \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y) + d(z_2, y)]^2 \\
 &\quad + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1 z_2 \in E(Q_\alpha(H_1)) \\ z_1 z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1) + d(z_2, y_2)]^2 = \sum_{B_1} + \sum_{B_2} + \sum_{B_3}.
 \end{aligned} \tag{30}$$

Now, we take

$$\begin{aligned}
 \sum_{B_1} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1), z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} [d(z_1, y_1) + d(z_2, y_2)]^2 \\
 &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1), z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_1) + d_{H_2}(y_1) + |V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right]^2 \\
 &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1), z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_1)^2 + d_{H_2}(y_1)^2 + |V(H_2)|^2 d_{Q_\alpha(H_1)}(z_2)^2 \right. \\
 &\quad \left. + 2|V(H_2)| d_{Q_\alpha(H_1)}(z_1) d_{H_2}(y_1) + 2|V(H_2)| d_{H_2}(y_1) d_{Q_\alpha(H_1)}(z_2) + 2|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_1) d_{Q_\alpha(H_1)}(z_2) \right] \\
 &= |V(H_2)|^4 F(H_1) + 2|V(H_2)| \|E(H_1)\| M_1(H_2) + 4|V(H_2)|^2 |E(H_2)| M_1(H_1) + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \\
 &\quad \times \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1), z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_2)^2 + \left(2|V(H_2)|^2 d_{H_1}(z_1) + 2|V(H_2)|^2 d_{Q_\alpha(H_1)}(z_1) \right) d_{Q_\alpha(H_1)}(z_2) \right].
 \end{aligned} \tag{31}$$

One can see that for a vertex $z_2 \in V(Q_\alpha(H_1)) - V(H_1)$, $d_{Q_\alpha(H_1)}(z_2) = d_{H_1}(z) + d_{H_1}(w)$, where $z_2 = xw \in E(H_1)$. Thus,

$$\begin{aligned}
 &= |V(H_2)|^4 F(H_1) + 2|V(H_2)| \|E(H_1)\| M_1(H_2) + 4|V(H_2)|^2 |E(H_2)| M_1(H_1) + \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \\
 &\quad \times \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1 \in V(H_1), z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)|^2 (d_{H_1}(z) + d_{H_1}(w))^2 + 2|V(H_2)|^2 (d_{H_1}(z_1) + d_{Q_\alpha(H_1)}(z_1)) (d_{H_1}(z) + d_{H_1}(w)) \right] \\
 &= |V(H_2)|^4 F(H_1) + 2|V(H_2)| \|E(H_1)\| M_1(H_2) + 4|V(H_2)|^2 |E(H_2)| M_1(H_1) \\
 &\quad + 2|V(H_2)|^4 HZ(H_1) + 2|V(H_2)|^4 (F(H_1) + 2M_2(H_1)) + 8|V(H_2)|^2 |E(H_1)| M_1(H_2) \\
 &= 2|V(H_2)|^4 HZ(H_1) + 3|V(H_2)|^4 F(H_1) + 12|V(H_2)|^2 |E(H_2)| M_1(H_1) \\
 &\quad + 2|V(H_2)| \|E(H_1)\| M_1(H_2) + 4|V(H_2)|^4 M_2(H_1), \\
 \sum_{B_2} &= \sum_{y \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1, z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_1) + |V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right]^2 \\
 &= 4(\alpha - 1) |V(H_2)|^2 \sum_{y \in V(H_2)} \sum_{uv \in E(H_1)} [d_{H_1}(u) + d_{H_1}(v)]^2 = 4(\alpha - 1) |V(H_2)|^3 HM(H_1), \\
 \sum_{B_3} &= \sum_{y_1 \in V(H_2)} \sum_{y_2 \in V(H_2)} \sum_{\substack{z_1, z_2 \in E(Q_\alpha(H_1)) \\ z_1, z_2 \in V(Q_\alpha(H_1)) - V(H_1)}} \left[|V(H_2)| d_{Q_\alpha(H_1)}(z_1) + |V(H_2)| d_{Q_\alpha(H_1)}(z_2) \right]^2 \\
 &= \alpha |V(H_2)|^4 \sum_{\substack{uv \in E(H_1) \\ vw \in E(H_2)}} [d_{H_1}(u) + d_{H_1}(v) + d_{H_1}(v) + d_{H_1}(w)]^2.
 \end{aligned} \tag{32}$$

TABLE 1: $P_n[P_m]$.

$[m, n]$	V	E	M_1	M_2	$F(H)$	$H(H)$
(3,3)	9	24	276	764	1704	3232
(4,4)	16	60	968	3868	8280	16 016
(5,5)	25	120	2460	12 576	26 460	51 612
(6,6)	36	210	5196	32 132	66 948	131 212
(7,7)	49	336	9716	70 276	145 488	286 040

TABLE 2: $P_{n(Q_a)}[P_m]$.

$[m, n, k]$	V	E	M_1	M_2	$F(H)$	$H(H)$
(3,3,3)	27	189	6366	53 701	114 786	222 188
(4,4,4)	64	944	69 024	1256 160	2745 760	5258 080
(5,5,5)	125	3175	392 030	$1.219\,569\,2 \times 10^7$	$2.581\,541 \times 10^7$	$5.020\,679\,4 \times 10^7$
(6,6,6)	216	8424	1561 992	$7.308\,936\,4 \times 10^7$	$1.522\,399\,68 \times 10^8$	$2.984\,186\,96 \times 10^8$
(7,7,7)	343	19 061	4939 998	$3.229\,925\,64 \times 10^8$	$6.663\,437\,62 \times 10^8$	$1.312\,328\,89 \times 10^9$

TABLE 3: Correlation coefficient between $P_{n(Q_a)}[P_m]$ and $P_n[P_m]$.

TI's	Value of R	Relationship between X and Y
First Zagreb index	0.9756	Very strong direct relationship
Second Zagreb index	0.953	Very strong direct relationship
Forgotten Zagreb index	0.9123	Very strong direct relationship
Hyper Zagreb index	0.9736	Very strong direct relationship

TABLE 4: Square of correlation coefficient between $P_{n(Q_a)}[P_m]$ and $P_n[P_m]$.

TI's	Value of R^2	Variability of Y is explained by X
First Zagreb index	0.9518	95.1 percent
Second Zagreb index	0.9080	90.8 percent
Forgotten Zagreb index	0.8323	83.23 percent
Hyper Zagreb index	0.9478	94.78 percent

FIGURE 5: Value of R for number of vertices, edges, first, second, forgotten, and hyper Zagreb indices. FIGURE 6: Value of R^2 for number of vertices, edges, first, second, forgotten, and hyper Zagreb indices.

W and X are the nodes of $L(H_1)$, so we have

$$\begin{aligned}
 &= \alpha |V(H_2)|^4 \sum_{WX \in E(L(H_1))} \left[d_{L(H_1)}(W)^2 + d_{L(H_1)}(X)^2 \right. \\
 &\quad \left. + 16 + 2d_{L(H_1)}(W)d_{L(H_1)}(X) + 8d_{L(H_1)}(W) + 8d_{L(H_1)}(X) \right] \\
 &= \alpha |V(H_2)|^4 \left[HZ(L(H_1)) + 8M_1(L(H_1)) + 16\left(\frac{1}{2}M_1(H_1) - E(H_1)\right) \right], \\
 \sum_{B_3} &= \alpha |V(H_2)|^4 [HZ(L(H_1)) + 8M_1(L(H_1)) + 8M_1(H_1) - 16E(H_1)].
 \end{aligned} \tag{33}$$

Consequently, the result is over. $\square$

3. Applications and Conclusion

For any two simple path graphs P_n and P_m with $n, m > 3$, we construct their lexicographic product graphs $P_n[P_m]$ and compute various degree-related TIs, as shown in Table 1 with certain values of m and n . Furthermore, we construct $Q_\alpha(P_n)$ by applying generalized line superposition operation on P_n and then construct Q_α -sum graph $(P_{n(Q_\alpha)}[P_m])$ based on lexicographic product of $Q_\alpha(P_n)$ and P_m . Finally, we compute certain degree-related TIs using Theorem 1–Theorem 4, as given in Table 2. We note that by the addition of vertices $\alpha \geq 1$, the values of obtained TIs are increasing for the newly constructed graphs comparatively to the graphs obtained by the ordinary lexicographic product of graphs.

3.1. Linear Regression Model. To check the correlation between the predefined lexicographic product of two simple graphs $(P_n[P_m])$ and newly defined Q_α -sum graphs $(P_{n(Q_\alpha)}[P_m])$, we have made the linear regression model for all the obtained indices as follows:

3.2. First Zagreb Index.

$$M_1(P_n[P_m]) = b_0 + b_1 \left[M_1(P_{n(Q_\alpha)}[P_m]) \right], \tag{34}$$

where $Y = M_1(P_n[P_m])$ index values, b_0 is the constant, b_1 is the regression coefficient, and $X = M_1(P_{n(Q_\alpha)}[P_m])$ index values (see Tables 1 and 2).

$$Y = 1207.7339 + 0.001805X. \tag{35}$$

3.3. Second Zagreb Index.

$$M_2(P_n[P_m]) = b_0 + b_1 \left[M_2(P_{n(Q_\alpha)}[P_m]) \right], \tag{36}$$

where $Y = M_2(P_n[P_m])$ index values, b_0 is the constant, b_1 is the regression coefficient, and $X = M_2(P_{n(Q_\alpha)}[P_m])$ index values (see Tables 1 and 2).

$$Y = 1548.9242 + 0.00002654X. \tag{37}$$

3.4. Forgotten Topological Index.

$$F(P_n[P_m]) = b_0 + b_1 \left[F(P_{n(Q_\alpha)}[P_m]) \right], \tag{38}$$

where $Y = F(P_n[P_m])$ index values, b_0 is the constant, b_1 is the regression coefficient, and $X = F(P_{n(Q_\alpha)}[P_m])$ index values (see Tables 1 and 2).

$$Y = 11263.1338 + 0.00008912X. \tag{39}$$

3.5. Hyper Zagreb Index.

$$HM(P_n[P_m]) = b_0 + b_1 \left[HM(P_{n(Q_\alpha)}[P_m]) \right], \tag{40}$$

where $Y = HM(P_n[P_m])$ index values, b_0 is the constant, b_1 is the regression coefficient, and $X = HM(P_{n(Q_\alpha)}[P_m])$ index values (see Tables 1 and 2).

$$Y = 30210.7664 + 0.0002023X. \tag{41}$$

Now, we represent a tabular representation of the correlation and square of correlation coefficient values related to the TIs of certain type of graphs $P_{n(Q_\alpha)}[P_m]$ and $P_n[P_m]$ (see Tables 3 and 4). The highest value of R and R^2 are indicated in bold.

For more explanation, see the graphical representation of correlation and square of correlation coefficient in Figures 5 and 6.

Data Availability

All the data are included within this paper. However, the reader may contact the corresponding author for more details of the data.

Conflicts of Interest

The authors have no conflicts of interest.

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