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DETOUR PADMAKAR IVAN INDICES OF HARMONIC GRAPHS

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Abstract

Graph theory is a fascinating and intellectually engaging area within the broader scope of Discrete Mathematics, providing abundant opportunities to explore a wide range of proof techniques. The concepts and findings from graph theory have far-reaching implications, making it a versatile tool with applications in various fields, including computer science, physics, biology, and social network analysis. This vast field of study classifies graphs based on particular structural characteristics. Specifically, a graph G is called a Pseudo-regular graph if all its vertices share the same average degree, indicating a consistent level of connectivity across the graph and resulting in a highly symmetric structure. In contrast, if the average degree of vertices varies across the graph, it is categorized as a Harmonic graph. Harmonic graphs feature a more intricate structure, where the degree of connectivity between vertices is not uniform. The differentiation between pseudo-regular and harmonic graphs underscores the diversity found within graph types and highlights the rich theoretical foundation that graph theory provides for the analysis of complex networks and structures. The Detour Padmakar-Ivan (DPI) of a graph G is defined as $DPI(G) = \sum_{e=uv\in E(G)} \left[N_u(e) + N_v(e)\right]$ and edges equidistant from both ends of the edges e = uv are not counted. Similar to the vertex version of Detour PI index, another important index Detour Co-PI index of G which is defined as $DCo-PI(G) = \sum_{e=uv\in E(G)} \left|N_u(e) - N_v(e)\right|$. In

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this paper computation of the Detour Pi , Detour Co-Pi Index in Harmonic graphs are proposed.

KEYWORDS*:* Detour Pi , Detour Co-Pi Index , Harmonic graphs.

1. Introduction

Throughout the paper, all of graphs are considered to be simple and connected. Let G = (V,E) be a simple connected graph. The vertex set and edge set of G denoted by V=V(G) and E=E(G), respectively. An edge e=uv of a graph G is joined between two vertices u and v. The distance between the vertices u and v of G is denoted by d(u,v) or $d_G(u,v)$ and defined as the number of edges in a shortest path connecting them.

A molecular graph or a chemical graph is a graph related to the structure of a chemical compound[6]. Each vertex of this graph represented an atom of the molecule and covalent bonds between atoms are represented by edges between the corresponding vertices[5].

A topological index of a graph is a single unique number characteristic of the graph and is mathematically invariant under graph automorphism[4]. In theoretical chemistry, the physico-chemical properties of chemical compounds are often modeled by the molecular graph based molecular structure descriptors, which are also referred to as topological indices[1].

It has been found to be a useful tool in QSAR (Quantitative structure-activity relationship) and QSPR(Quantitative structure -property relationship)[7]. Quantitative structure- activity relationship (QSAR) are mathematical models designed for the correlation of various types of biological activity, chemical reactivity, equilibrium, physical and physicochemical properties with electronic, steric, hydrophobic and other factors of a molecular structure of a given series of compounds such as substitution constants, topological indices (TI) as well as with solvent and other physicochemical parameters.

The detour index provides information about the overall connectivity and distance properties of a graph. A higher detour index indicates that the graph has longer average distances between pairs of vertices, while a lower detour index indicates that the graph is more tightly connected. The detour index can be useful in various applications, such as in studying network communication efficiency, analyzing transportation networks, or understanding the overall structure of a graph. It complements other topological indices and can provide additional insights into the properties of a graph.

The Padmakar-Ivan(PI) index of a graph G is the sum over all edges uv of G of the number of edges which are not equidistant from the vertices u ad v. The CO-PI index of G is defined as $\text{CO-PI}_v(G) = \sum_{e=uv\in E(G)} \left| n_u(e) - n_v(e) \right|$.

The Detour Padmakar-Ivan (DPI) of a graph G is defined as $DPI(G) = \sum_{e=uv\in E(G)} \left[N_u(e) + N_v(e) \right]$ and edges equidistant from both ends of the edges e = uv are not counted.

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Similar to the vertex version of Detour PI index, another important index Detour Co-PI index of G which is defined as $DCo-PI(G) = \sum_{e=uv\in E(G)} \left| N_u(e) - N_v(e) \right|$

The Padmakar Ivan Index has several important applications, particularly in the fields of chemistry and molecular design. It is commonly used to predict the chemical and physical properties of molecules, aiding in the identification of their behavior and characteristics. Additionally, it plays a crucial role in the design of new molecules with specific, desired properties, contributing to the creation of compounds tailored for particular functions. This index is also valuable in the analysis of molecular graphs within computational chemistry, where it helps researchers understand the structure of molecules. What makes the Padmakar Ivan Index especially useful is its focus on the overall connectivity of atoms in a molecule, rather than just considering individual atoms or bonds, making it an effective tool for examining the intricate relationships that define molecular structures. A graph G is called Harmonic graph(Pseudo-regular graph) [13] if every vertex of G has equal average degree .The main goal of this paper is to find the Detour Pi and Detour Co-Pi index of Harmonic graphs .

2. HARMONIC GRAPHS

Let G= (V, E) be a simple, connected undirected graph with n vertices and m edges. For any vertex $v_i \in V$, the degree of v_i is the number of edges incident on v_i. It is denoted by d_i or d (v_i)

In a regular graph, every vertex has the same degree, meaning each vertex is incident to the same number of edges. The degree of a vertex in a graph is the number of edges incident to that vertex.

Formally, a graph G = (V,E) is called k-regular if every vertex in V has degree k, wherek is a non-negative integer. So, in a k-regular graph, every vertex is incident to exactly k edges.

A semi-regular bipartite graph is a specific type of bipartite graph in which all the vertices within the same part of the bipartition have the same degree. To clarify, a bipartite graph is a type of graph where the set of vertices can be divided into two distinct, disjoint sets, with the key property that no two vertices within the same set are adjacent to each other. In other words, edges only exist between vertices belonging to different sets, and no edges connect vertices within a single set. In the case of a semi-regular bipartite graph, the vertices in one of these sets will each have the same number of connections (or edges) to vertices in the other set, thus ensuring uniformity in the degree of vertices within each part of the bipartition.

In a semiregular bipartite graph, each vertex within one part has the same degree, meaning they are all incident to the same number of edges, but the degrees may differ between the two parts.

This property makes semiregular bipartite graphs particularly interesting in various applications, especially in modeling systems where different entities interact in a structured way.

The 2-degree of v_i [13] is the sum of the degree of the vertices adjacent to v_i and denoted by

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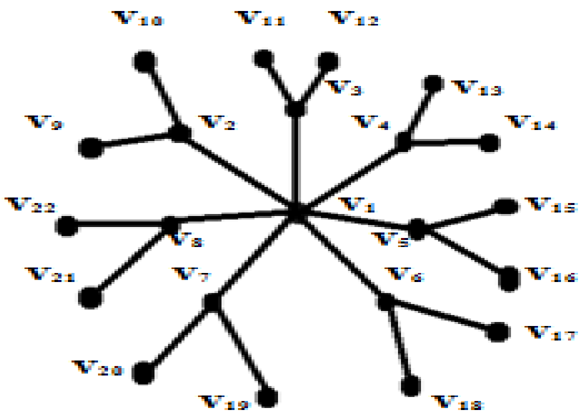
t_i.[11]. The average degree of v_i is defined as t_i/d_i. For any vertex $v_i \in V$, the average degree of v_i is also denoted by $m(v_i) = t_i/d_i$.

A graph G is called Harmonic graph(Pseudo-regular graph) [16] if every vertex of G has equal average degree and $m(G) = \frac{1}{n}\sum_{v \in V(G)} m(u)$ is the average neighbor degree number of the graph G.

A graph is said to be r-regular if all its vertices are of equal degree r. Every regular graph is a Harmonic graph [17]. But the Harmonic graph need not be a regular graph. Harmonic graph is shown in the following figure (1) and figure (2).



Fig(1)

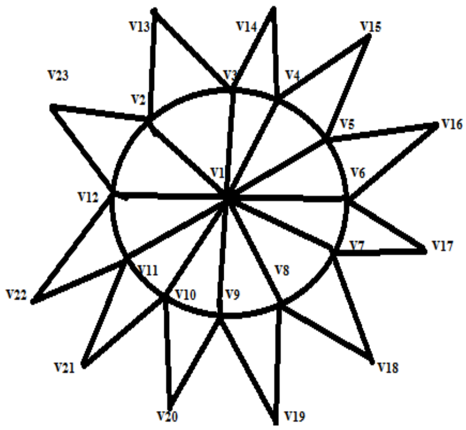


Fig-2

In Figure-1, there are 14 vertices are of degree 1, 7 vertices of degree 3 and 1 vertex is of degree 7. So totally there are 22 vertices in the graph. Average degree of vertices of degree 1 is equal to 3/1 = 3. Average degree of vertices of degree 2 is equal to 9/3 = 3. Average degree of vertices of degree 7 is equal to 21/7=3. Therefore, Average degree of each vertex is 3. Hence it is a Harmonic graph. In Figure-2, average degree of each vertices is 5. Hence the graph in the Figure -2 is also a Harmonic graph.

Indeed, Harmonic graphs serve as intriguing models for understanding the structure and behavior of complex networks in various domains. Here's a bit more details on related to

Balance between regularity and randomness: Harmonic graphs exhibit a unique structural balance that lies between the well-defined, predictable structure of regular graphs, where every vertex has the same degree, and the unpredictable, arbitrary nature of random graphs, where edges are distributed without any specific pattern or rules. This intermediate structure in harmonic graphs strikes a balance between order and randomness, providing a fascinating framework for researchers to investigate and understand how various network properties and behaviors emerge when the graph's structure is neither completely uniform nor entirely random. By studying harmonic graphs, researchers can gain insights into how networks

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function and evolve when their structural properties are influenced by a combination of both regularity and randomness.

Real-world applicability : In real-world scenarios, many complex networks, including social networks, biological networks (such as protein-protein interaction networks), and communication networks, often display characteristics that resemble pseudo-regularity. These networks typically feature elements of consistency in their structure, with certain aspects of connectivity maintaining uniformity, though not to the extent of full regularity. By examining harmonic graphs, researchers are able to gain a deeper understanding of the dynamics and processes that drive the formation and functioning of such networks. Through the study of these graphs, researchers can uncover the intricate underlying mechanisms that influence how connections are made, how information flows, and how relationships evolve within these real-world networks. This exploration helps to provide valuable insights into the balance between structure and randomness that governs many of the networks we encounter in various domains, from social interactions to biological systems.

Complexity : The study of harmonic graphs introduces a higher level of complexity to traditional graph theory by blending deviations from strict regularity with certain maintained structural properties. Unlike purely regular graphs, which have uniform vertex degrees, or purely random graphs, which lack consistent patterns, harmonic graphs occupy a middle ground. This intermediate structure allows researchers to explore and identify patterns and phenomena that may not be immediately visible in graphs that are completely regular or entirely random. By analyzing harmonic graphs, it becomes possible to uncover unique behaviors and dynamics that arise from the combination of regularity and randomness, thus offering new insights into network structures that cannot be observed in simpler graph types. The added complexity of harmonic graphs provides a richer understanding of how networks can function and evolve.

Robustness and resilience : Understanding the robustness and resilience of Harmonic networks involves analyzing how these networks behave when subjected to disturbances, perturbations, or deliberate targeted attacks. By studying their response mechanisms, we can gain deeper insights into the structural and functional integrity of such networks under stress. This comprehensive understanding is crucial for enhancing the design of networks that are not only strong but also capable of recovering from disruptions. Such knowledge plays a vital role in developing more resilient systems across a wide range of practical domains, including but not limited to communication systems, transportation infrastructures, energy grids, and other critical networked environments. By applying these insights, engineers and researchers can build networks that maintain operational continuity and performance, even in the face of unexpected failures or malicious threats.

Algorithm development : Harmonic graphs pose interesting challenges for algorithm development, particularly for tasks such as network optimization, community detection, and information diffusion. Developing efficient algorithms for analyzing and manipulating Harmonic graphs can have practical implications in various domains.

In summary, the study of Harmonic graphs enriches our understanding of complex networks by providing a middle ground between regular and random graphs, offering insights into real-world systems' structure and behavior, and posing intriguing challenges for theoretical and practical research.

Overall, the applications of Pseudo-regular graphs span multiple domains, offering valuable insights into the structure, behavior, and optimization of complex networks. By leveraging the unique properties of Pseudo-regular graphs, researchers can advance their understanding of network dynamics and develop innovative solutions for a wide range of practical challenges.

The relevance of Harmonic graph for the theory of nanomolecules and nanostructure should become evident from the following[15]. There exist Polyhedral(planar, 3-connected) graphs and infinite periodic planar graphs belonging to the family of the Harmonic graphs. Among polyhedral, the deltoidal hexecontahedron possesses Harmonic property. The deltoidal hexecontahedron is a Catalan polyhedron with 60 deltoid faces, 120 edges and 62 vertices with degree 3,4 and 5 and average degree of its vertices is 4.

A variety of their chemically relevant polyhedral and polyhedral-type structure, whose graphs are Pseudo-regular, can be found in the book [13,14]. In this paper, the Harmonic graphs can be drawn based on the value of average degree p(say) only.

3. CONSTRUCTION OF HARMONIC GRAPHS (PSEUDO-REGULAR GRAPH):

In this section algorithms are proposed to construct Harmonic graphs.

A. Algorithm to construct the Harmonic graph of type I denoted by G_I

Step1: For any positive integer $p \geq 2$, draw a star graph $G = K_{1,m}$ where $m=p^2-p+1$.
Let v_0 be the central vertex of G and let $v_1, v_2, \ldots, v_m$ be the n pendant vertices.
Step 2: Join (p-1) new pendant vertices to every vertex of G except the central vertex.
Step3: The new resulting graph is a Harmonic graph of type I. It is denoted by
G_I.

$|V(G_I)| = 1+p^2-p+1+(p-1)(p^2-p+1)$
$= 1+p^2-p+1+p^3-p^2+p-p^2+p-1$
$= p^3-p^2+p+1$
$|E(G_I)| = (p^2-p+1) + (p-1)(p^2-p+1)$
$= p^3-p^2+p$

G_I is a tree for any positive constant p and average degree of each vertex is p.
G_I type Harmonic graph is given in Figure-1.

B. Algorithm to construct the Harmonic graph of type II denoted by G_{II}

Step 1: For any positive integer $p \geq 3$, draw a wheel graph K_1+C_m with m spokes, where $m = p^2 - 3p + 3$. Let v_o be the central vertex of W_{m+1} and hence $d(v_0) = p^2-3p+3$.
Step 2: Let $\{v_1, v_2, \ldots, v_m\}$ be the vertices of the cycle in C_m. Join p-3 pendant Vertices to every vertex in the cycle except the central vertex. The resulting

graph is a type II Harmonic graph . It is denoted by G_{II}.

Step 3: $|V(G_{II})| = p^3-3p+3+1+(p-3)(p^2-3p+3)$

$= p^3-5p^2+9p-5$

For p=5, we can get the following Harmonic graph

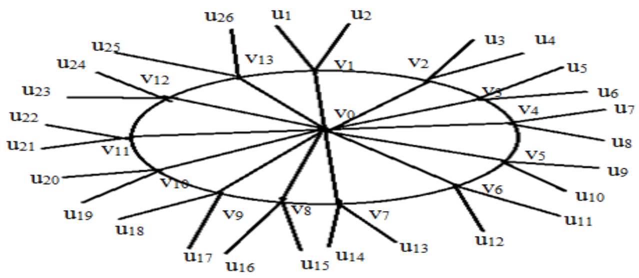

Fig-3

C. Algorithm to construct the Harmonic graph of type III denoted by G_{III}

Step 1: For any positive integer $p \geq 5$, draw a wheel graph $K_1 + C_m$ with m spokes, where $m = p^2-3p+1$. Let v_o be the central vertex of wheel graph and hence $d(v_o) = p^2-3p+1$.

Step 2: Let $\{v_1, v_2, \ldots, v_m\}$ be the vertices of the cycle in C_m. Introduce a new vertex for each edge of the cycle in a wheel graph and every new vertices should be joined to the end vertices of each edge of a cycle.

Step 3: Join (p-5) pendant vertices to every vertex of the cycle in the wheel graph except the central vertex. $|V(G_{III})| = p^3-6p^2+10p-2$. The resulting graph is Harmonic graph of type III. It is denoted by G_{III}.

For p=6, we can get the following Harmonic graph

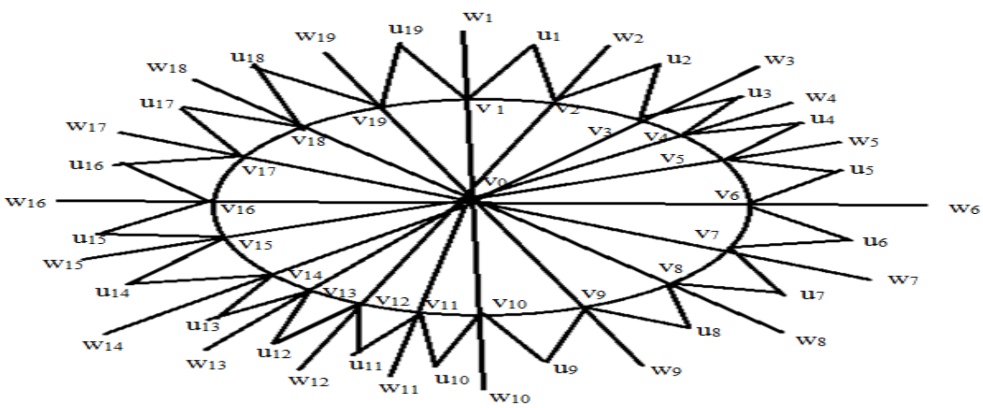

Fig-4

4. MAIN RESULTS:

4.1 Detour PI and Detour Co-PI index of Harmonic graphs

The Detour Padmakar-Ivan (DPI) of a graph G is defined as $DPI(G) = \sum_{e=uv \in E(G)} \left[N_u(e) + N_v(e) \right]$ and edges equidistant from both ends of the edges e =

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uv are not counted. Similar to the vertex version of Detour PI index, another important index Detour Co-PI index of G which is defined as $DCo-PI(G) = \sum_{e=uv\in E(G)} \left|N_u(e) - N_v(e)\right|$

Theorem 4.1.1: For p ≥ 2, the DPI index of type I Harmonic graph G_I is

$DPI(G_I) = P(P^2 - P + 1)|-P^3 + P^2 - P - 1|$

Proof: Let $G = G_I$ be a type I Pseudo-regular graph.

Let $V(G) = \{v_0, v_1, v_2, \ldots, v_m, u_1, u_2, \ldots, u_{m(p-1)}\}$ be the vertex set of G and v_0 as the central vertex of $K_{1,m}$ and $\{v_1, v_2, \ldots, v_m\}$ are pendant vertices of $K_{1,m}$ where $m = p^2-p+1$ and the (p-1) pendant vertices $\{u_1, u_2, \ldots, u_{m(p-1)}\}$ are attached with m pendant vertices $v_1, v_2, \ldots, v_m$.

Let $E(G) = (v_0v_i;\ 1 \le i \le m\}$ U $\{v_1u_j;\ 1 \le j \le p-1\}$ U$\{v_2u_j;\ p \le j \le 2p-2\}$ U$\{v_3u_j;\ 2p-1 \le j \le 3p-3\}$U……….$\{v_mu_j;\ (m-1)p-m+2 \le j \le mp-m\}$.The Harmonic graph with p=3 is shown in Fig-1

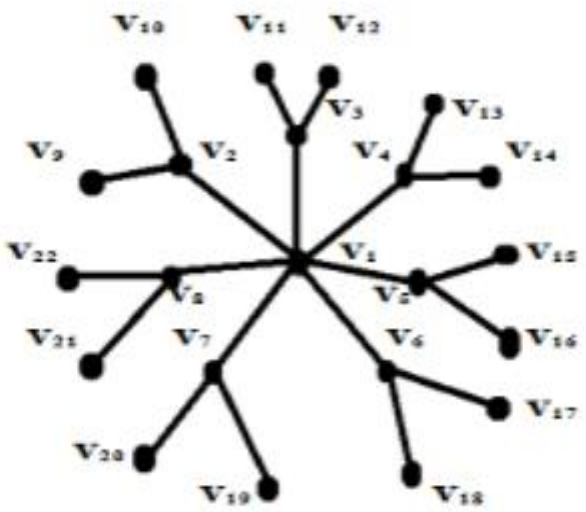

Fig-1

The DPI index of G is given by $DPI(G) = \sum_{e=uv\in E(G)} \left|N_u(e) + N_v(e)\right|$

$$PI(G_I) = \sum_{e=uv\in E(G)} \left|N_u(e) + N_v(e)\right|$$

$$= \sum_{\text{pendant edge } e\in E(G)} \left|N_u(e) + N_v(e)\right| + \sum_{\text{non pendant edge } e\in E(G)} \left|N_u(e) + N_v(e)\right|$$

$$= (p-1)(p^2-p+1)\left|1-(p(p^2-p+1)+1+1)\right| + (p^2-p+1)\left|p-(p(p^2-p+1)+1-p\right|$$

$$= (p^2-p+1)\left[\left|-p^3+p^2-p-1\right|(p-1+1)\right]$$

$$= p(p^2-p+1)\left|-p^3+p^2-p-1\right|$$

Now

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Theorem 4.1.2: For p ≥ 2, the DCO-PI index of type I Harmonic graph G_I is $DCOPI(G_I) = (P^2 - P + 1)\left((P-1)\left|-P^3 + P^2 - P + 1\right| + \left|-P^3 + P^2 + P - 1\right|\right)$

Proof: Similar to theorem 4.1.1,

The DCO-PI index of G is given by $DCO-PI(G) = \sum_{e=uv\in E(G)} \left|N_u(e) - N_v(e)\right|$

$$\begin{aligned}
DCO\text{-}PI(G_I) &= \sum_{e=uv\in E(G)} \left|N_u(e) - N_v(e)\right| \\
&= \sum_{\text{pendant edge } e\in E(G)} \left|N_u(e) - N_v(e)\right| + \sum_{\text{non pendant edge } e\in E(G)} \left|N_u(e) - N_v(e)\right| \\
&= (p-1)(p^2 - p + 1)\left|1 - (p(p^2 - p + 1) + 1 - 1)\right| + (p^2 - p + 1)\left|p - (p(p^2 - p + 1) + 1 - p\right| \\
&= (p-1)(p^2 - p + 1)\left|1 - p^3 + p^2 - p\right| + (p^2 - p + 1)\left|p - p^3 + p^2 - 1\right| \\
&= (p^2 - p + 1)\left[(p-1)\left|-p^3 + p^2 - p + 1\right| + \left|-p^3 + p^2 + p - 1\right|\right]
\end{aligned}$$

Now

Theorem 4.1.3: Let G = G_{II} be a type II Harmonic graph. Then $DPI(G) = m(p^4 - 8p^3 + 24p^2 - 29p + 10)$ and $DCo-PI(G) = m(p-3)(p^3 - 5p^2 + 9p - 8)$ for p ≥ 3

Proof:

The vertex set V(G) and the edge set E(G) are described as in theorem 2.3.2.

$$DPI(G) = \sum_{e=uv\in E(G)} \left[N_u(e) + N_v(e)\right]$$

$$= \sum_{i=1}^{m} D(v_0, v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} D(v_i, v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-3)} D(v_i, u_j)$$

y definition,

$$= m[1 + (p-2)] + m[(p-2) + (p-2)] + m(p-3)[(p^3 - 5p^2 + 9p - 6) + 1]$$

and

$$= m[p - 1 + 2p - 4 + (p-3)(p^3 - 5p^2 + 9p - 5)]$$

$$= m(p^4 - 8p^3 + 24p^2 - 29p + 10)$$

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$$DCo-PI(G) = \sum_{e=uv\in E(G)} \left|N_u(e)-N_v(e)\right|$$

$$= \sum_{i=1}^{m} D(v_0,v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} D(v_i,v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-3)} D(v_i,u_j)$$

$$= m\left[1-(p-2)\right] + m\left[(p-2)-(p-2)\right] + m(p-3)\left[(p^3-5p^2+9p-6)-1\right]$$

$$= m\left[3-p+(p-3)(p^3-5p^2+9p-7)\right]$$

$$= m(p-3)(p^3-5p^2+9p-8)$$

Theorem 4.1.4: Let G = G_{III} be a III Harmonic graph. Then $DPI(G) = m\left[m(p-3)(p-2)+3p-10\right]$ and $DCo-PI(G) = m(p-4)\left[m(p-3)-1\right]$ for p ≥ 5.

Proof:

The vertex set V(G) and the edge set E(G) are described as in theorem 2.3.3.

By definition,

$$DPI(G_{III}) = \sum_{e=uv\in E(G)} \left[N_u(e)+N_v(e)\right]$$

$$= \sum_{i=1}^{m} D(v_0,v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} D(v_i,v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m} D(v_i,u_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-5)} D(v_i,w_j)$$

$$= m\left[1+m(p-3)\right] + m\left[(p-4)+(p-4)\right] + m(p-5)\left[m(p-3)+1\right] + 2m\left[m(p-3)+1\right]$$

$$= m\left[3m(p-3)+2p-5+(p-5)m(p-3)+(p-5)\right]$$

$$= m\left[m(p-3)(p-2)+3p-10\right]$$

And

$$DCo-PI(G) = \sum_{e=uv\in E(G)} \left|N_u(e)-N_v(e)\right|$$

$$= \sum_{i=1}^{m} D(v_0,v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} D(v_i,v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m} D(v_i,u_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-5)} D(v_i,w_j)$$

$$= m\left[1-m(p-3)\right] + m\left[(p-4)-(p-4)\right] + m(p-5)\left[m(p-3)-1\right] + 2m\left[m(p-3)-1\right]$$

$$= m\left[m(p-3)-1+(p-5)m(p-3)-(p-5)\right]$$

$$= m(p-4)\left[m(p-3)-1\right]$$

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