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On Bounds for the Energy and Arithmetic Geometric Radius of Apéry Poset Graphs

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Abstract. The energy and arithmetic-geometric radius are two important indices used to measure the network complexity, molecular properties, connectivity and stability of graphs. In this article, several parameters of Apéry poset graphs have been computed. Moreover, based on these graph parameters, some sharp bounds for the energy and arithmetic-geometric radius have been given.

AMS (MOS) Subject Classification Codes: 05C25, 06A11, 11D72
Key Words: Numerical semigroup, Apéry poset, Order and size of graph.

1. Introduction and preliminaries

Consider a chemist conducting a multi step reaction in which several reagents interact to yield two final products, one of which is undesirable. During the process, a number of unstable intermediates are formed, and their interactions determine the eventual outcome of the reaction. The structure of the Apéry poset graph provides a natural model for this system, where the elements of Apéry poset represent the unstable intermediates, while an edge between two elements corresponds to the possibility of their combination producing a stable compound within the semigroup. The energy of the Apéry poset graph then reflects the overall reactivity of the system, capturing the extent and strength of possible interaction pathways. By analyzing this energy and the connectivity patterns of the graph, the chemist can identify which reaction routes are more likely to yield undesired products. Adjusting reaction conditions or introducing selective reagents corresponds, in graph theocratic terms, to restricting certain edges or redirecting connections, thereby guiding the system toward the desired product. In this way, the Apéry poset graph framework offers a mathematical perspective for understanding and optimizing complex chemical reaction networks.
Graph theory is a branch of mathematics that focuses on studying the objects formed by vertices interconnected through edges. Originally emerging from recreational mathematical challenges, this field has developed into a crucial area of mathematical research, with applications spanning numerous fields, including chemistry, operations research, social sciences, and computer science. [2, 6, 13, 18]. This domain allows researchers to examine a network of nodes and links, which can symbolize a variety of entities, including urban

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layouts and digital data, to ascertain the most effective pathways. It uses social network analysis, the prioritization of hyperlinks in search engines, and GPS navigation for determining the most efficient route.
Let $\mathfrak{G}$ denote a graph defined by its set of vertices and set of edges, denoted by $V(\mathfrak{G})$ and $E(\mathfrak{G})$, respectively. The $|V(\mathfrak{G})|$ and $|E(\mathfrak{G})|$, in a graph is known as the order and the size of graph. The degree of a vertex is characterized by the total number of edges connected to it. Furthermore, within the framework of a graph $\mathfrak{G}$, the notations $\delta(\mathfrak{G})$ and $\Delta(\mathfrak{G})$ denote the minimum and maximum degrees, respectively. Arithmetic-Geometric matrix of Graph $\mathfrak{G}$ is denoted by $A_{ag}[\mathfrak{G}]$ and is defined as $A_{ag}[\mathfrak{G}] = (b_{ij})$. Where $b_{ij} = \frac{(d_{u_1}+d_{u_2})}{2\sqrt{d_{u_1}d_{u_2}}}, u_1, u_2 \in E(\mathfrak{G})$ and zero otherwise. Eigenvalues of $A_{ag}[\mathfrak{G}]$ is denoted by $\mu_{ag}^1 \geq \mu_{ag}^2 \geq ... \geq \mu_{ag}^m$, , where μ_{ag}^1 is called the Arithmetic Geometric Spectral Radius of $\mathfrak{G}$. The Arithmetic Geometric Energy is defined as $\mathfrak{E}_{ag} = \sum_{i=1}^{m} |\mu_{ag}^i|$. For more details, see [4, 5, 12, 19].
Chemical graph theory is a specialized area within graph theory that concentrates on the analysis of molecular structures and chemical compounds through the application of graph-theoretical principles and methodologies. By utilizing graphs, one can effectively represent key characteristics of molecular structures and investigate their influence on various chemical properties and behaviors. In the context of graph theory, the configuration of a graph, denoted by a numerical value, is known as the topological index. Numerous notable topological indices that are determined exclusively by the vertex degrees of the graph under consideration are particular cases of the subsequent graph invariant:

$$BID(\mathfrak{G}) = \sum_{w_i w_j \in \mathrm{E}} g(d_{w_i}, d_{w_j}),$$

In this context, g represents a non-negative, real-valued symmetric function, and the topological indices expressed in terms of this symmetric function are commonly known as bond incident degree indices, abbreviated as BID indices. Table 1 presents the g-functions associated with several important topological indices that will be referenced in the subsequent sections. Several topological indices are listed in Table 1, which are used to find bounds for the arithmetic-geometric radius and arithmetic-geometric energy.

Table 1 Some Topological Indices

Function $g(d_{w_i}, d_{w_j})$	Equation (1) pertains to	Symbol
$(d_{w_i} + d_{w_j})$	First Zagreb index [7]	$M_1[\mathfrak{G}]$
$\frac{1}{d_{w_i}d_{w_j}}$	Modified second Zagreb index [14]	$Z[\mathfrak{G}]$
$(d_{w_i})^2 + (d_{w_j})^2$	Forgotten index [7]	$F[\mathfrak{G}]$
$(d_{w_i}d_{w_j})$	Second Zagreb index [8]	$M_2[\mathfrak{G}]$
$(d_{w_i}d_{w_j})^{\frac{-1}{2}}$	Randić index [15]	$R_{\frac{-1}{2}}[\mathfrak{G}]$

A numerical semigroup Υ is a cofinite submonoid of the additive monoid of positive integers $\mathbb{N}$, including 0. The smallest positive number in the set Υ is referred to as the multiplicity of Υ, denoted by α. The set difference $g(\Upsilon) = \mathbb{N} \setminus \Upsilon$ is the gap set of Υ, and the greatest element within the set $g(\Upsilon)$ is the Frobenius number, denoted by $\Im$. Let

$X = \{a_1, a_2, \ldots, a_n\}$ be a system of generators of Υ, then $\Upsilon = \langle X \rangle$. The set X is referred to as the minimal set of generators if no proper subset of X can generate Υ, and its cardinality is denoted by $e(\Upsilon)$. Furthermore, if $\Im - a \in \Upsilon$ for every $a \in g(\Upsilon)$, then Υ is known as symmetric [1, 16].
In section 2, we compute size and degree sequences of Apéry poset graph. In section 3, we compute the First Zagreb index, Modified second Zagreb index, Forgotten index, Second Zagreb index and Randić index. Moreover on the basis of these graph parameters and topological indices, we found bounds for the arithmetic-geometric radius and arithmetic-geometric energy.

2. The Size and Degree Sequence of Apéry Poset Graphs

The Apéry set with respect to the multiplicity α of a numerical semigroup Υ, is defined as

$$\mathcal{P} = \mathfrak{A}_{\mathcal{P}}(\Upsilon, \alpha) = \{s \in \Upsilon : s - \alpha \notin \Upsilon\}.$$

Let $s_1, s_2 \in \mathcal{P}$, then $s_2 \prec_\Upsilon s_1$ if and only if $s_1 - s_2 \in \Upsilon$. It is easy to see that $(\mathcal{P}, \prec_\Upsilon)$ is a poset. An Apéry poset graph is an undirected simple graph $\mathfrak{G}_{\mathcal{P}}$ such that

$$\mathrm{V}(\mathfrak{G}_{\mathcal{P}}) = \{u_x : x \in \mathfrak{A}_{\mathcal{P}}(\Upsilon, \alpha)\},$$

$$\mathrm{E}(\mathfrak{G}_{\mathcal{P}}) = \{u_x u_y : x - y \in \Upsilon \ \ or \ \ y - x \in \Upsilon\}.$$

In this paper, we consider Apéry poset graphs associated with the following infinite class of symmetric numerical semigroups having arbitrary multiplicity and embedding dimension:

$$\Upsilon = \langle \alpha, \alpha + 1, q\alpha + 2q + 2, ..., q\alpha + \alpha - 1\rangle, \alpha = 2q + e, q \in \mathbb{N}.$$

The Frobenius number F for this class is $2q\alpha + 2q + 1$.

Lemma 2.1. *The graph $\mathfrak{G}_{\mathcal{P}}$ is a tri-degreed graph that has $(e-2)$ number of vertices with degree 2, two vertices with degree $\alpha - 1$ and $2q$ number of vertices with degree $2q + 1$.*

Proof. From [17], we have

$$\begin{aligned}\mathfrak{A}_{\mathcal{P}}(\Upsilon, \alpha) = \{\, & 0 < \alpha + 1 < 2\alpha + 2 < \cdots < q\alpha + q \\ & < q\alpha + 2q + 2 < q\alpha + 2q + 3 < \cdots < q\alpha + \alpha - 1 \\ & < (q+1)\alpha + q + 1 < (q+2)\alpha + q + 2 < \cdots \\ & < (2q+1)\alpha + 2q + 1 \,\}.\end{aligned}$$

We can write, $\mathfrak{A}_{\mathcal{P}}(\Upsilon, \alpha) = X \cup Y$, where

$$X = \{k(\alpha + 1), 0 \leq k \leq 2q + 1\}, \ \ Y = \{q\alpha + 2q + b, 2 \leq b \leq \alpha - 1 - 2q\}.$$

For $k_1 < k_2$, we have

$$k_2(\alpha+1) - k_1(\alpha+1) = (k_2 - k_1)(\alpha+1) \in \Upsilon.$$

This implies that the induced subgraph $\mathfrak{G}_{\mathcal{P}}[X]$ of $\mathfrak{G}_{\mathcal{P}}$ is a complete graph K_{2q+2}. Since Y is contained in the minimal generating system, therefore the induced subgraph $\mathfrak{G}_{\mathcal{P}}[Y]$ of $\mathfrak{G}_{\mathcal{P}}$ is an edgeless graph. Note that for $1 \leq k \leq q$,

$$q\alpha + 2q + b - k(\alpha+1) = (q-k)\alpha + 2q + b - k.$$

Since $\max\{2q+b-k\} = \alpha - 1$ and $2q + b - k > (q-k)$. Therefore, by Lemma 1 of [9], we have

$$q\alpha + 2q + b - k(\alpha+1) = (q-k)\alpha + 2q + b - k \notin \Upsilon.$$

Also, for $q+1 \leq k \leq 2q$,

$$\begin{aligned} F - \big(k(\alpha+1) - (q\alpha+2q+b)\big) &= 2q\alpha + 2q + 1 - k(\alpha+1) + q\alpha + 2q + b \\ &= 2q\alpha + 2q + 1 - k\alpha - k + q\alpha + 2q + b \\ &= (2q-k)\alpha + (2q-k) \\ &\quad + (q\alpha + 2q + b + 1). \end{aligned}$$

Note that $(2q-k)\alpha + (2q-k) \in \Upsilon$, by Lemma 1 of [9] and since $(q\alpha + 2q + b + 1)$ is contained in the minimal generating system, therefore

$$F - (k(\alpha+1) - (q\alpha+2q+b)) \in \Upsilon,$$

which implies that $k(\alpha+1) - (q\alpha+2q+b) \notin \Upsilon$. Since

$$(2q+1)\alpha + 2q + 1 - (q\alpha + 2q + b) = q\alpha + \alpha + 1 - b \in \Upsilon,$$

therefore the vertices corresponding to $(2q+1)\alpha+2q+1$ and 0 has maximum degree $\alpha-1$. As $|X|=2q+2$ and $|Y|=\alpha-2q-2$, therefore $2q$ vertices have degree $2q+1$, $\alpha-2-2q$ vertices have degree 2. □

Proposition 2.2. *The size of the graph $\mathfrak{G}_{\mathcal{P}}$ is $|\mathrm{E}(\mathfrak{G}_{\mathcal{P}})| = 2\alpha-3-q+2q^2$. Moreover, the partition of edges according to the degree of end vertices of graph $\mathfrak{G}_{\mathcal{P}}$ is shown in the following Table 2.*

Table 2 Partition of edges according to the degree of end vertices

	(d_{w_i}, d_{w_j}) *Where* $w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})$	*Number of Edges*
E_1	$(\alpha-1, \alpha-1)$	1
E_2	$(2q+1, 2q+1)$	$\frac{2q(2q-1)}{2}$
E_3	$(2q+1, \alpha-1)$	$4q$
E_4	$(2, \alpha-1)$	$2(e-2)$

Proof. This follows from Lemma 2.1. □

3. Arithmetic Geometric Spectral Radius of Apéry Poset Graphs

In this section, we compute some bounds of Arithmetic Geometric Spectral Radius of Graph $\mathfrak{G}_{\mathcal{P}}$.

Lemma 3.1. [20] *If R is an $i \times i$ real symmetric matrix with eigenvalues $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_i$, then for any $0 \neq y \in \mathbf{R^i}$, $y^tRy \leq \mu_1 y^t y$. Moreover, equality holds $\Leftrightarrow$ y is eigenvector of R corresponding to μ_1.*

Theorem 3.2. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$\mu^1_{ag}[\mathfrak{G}_{\mathcal{P}}] \geq \frac{4(2\alpha-3-q+2q^2)}{\alpha(\alpha-1)}.$$

Proof. Let $Y = (y_1, y_2, ..., y_{q\alpha+q+1})^t$ be a unit vector in $\mathbf{R}^\alpha$. Therefore by Lemma 3.1

$$\mu^1_{ag}[\mathfrak{G}_{\mathcal{P}}] \geq Y^t A_{ag}[\mathfrak{G}_{\mathcal{P}}]Y = \sum_{w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} \frac{d_i[\mathfrak{G}_{\mathcal{P}}] + d_j[\mathfrak{G}_{\mathcal{P}}]}{\sqrt{d_i[\mathfrak{G}_{\mathcal{P}}]d_j[\mathfrak{G}_{\mathcal{P}}]}} y_iy_j \geq \frac{4}{\alpha - 1} \sum_{w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} y_iy_j.$$

Put $Y = \left(\frac{1}{\sqrt{\alpha}}, \frac{1}{\sqrt{\alpha}}, ..., \frac{1}{\sqrt{\alpha}}, \right)^t$ in the above expression, we get

$$\mu^1_{ag}[\mathfrak{G}_{\mathcal{P}}] \geq Y^t A_{ag}[\mathfrak{G}_{\mathcal{P}}]Y \geq \frac{4(2\alpha - 3 - q + 2q^2)}{\alpha(\alpha - 1)}.$$

□

Theorem 3.3. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$\mu^1_{ag}[\mathfrak{G}_{\mathcal{P}}] \leq \frac{\alpha - 1}{2} \mu^1[\mathfrak{G}_{\mathcal{P}}].$$

Proof. Let $Y = (y_1, y_2, ..., y_\alpha)^t$ be a unit vector in $A_{ag}[\mathfrak{G}_{\mathcal{P}}]$ corresponding to eigenvalue $\mu^1_{ag}[\mathfrak{G}_{\mathcal{P}}]$. Then

$$\begin{aligned} \mu^1_{ag}[\mathfrak{G}_{\mathcal{P}}] = Y^t A_{ag}[\mathfrak{G}_{\mathcal{P}}]Y &= \sum_{w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} \frac{d_i[\mathfrak{G}_{\mathcal{P}}] + d_j[\mathfrak{G}_{\mathcal{P}}]}{\sqrt{d_i[\mathfrak{G}_{\mathcal{P}}]d_j[\mathfrak{G}_{\mathcal{P}}]}} y_iy_j \\ &\leq \frac{2(\alpha - 1)}{2} \sum_{w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} y_iy_j. \end{aligned}$$

Again by Lemma 3.1

$$\mu^1[\mathfrak{G}_{\mathcal{P}}] \geq Y^t A[\mathfrak{G}_{\mathcal{P}}]Y = 2 \sum_{w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} y_iy_j.$$

By combining the above expressions, we obtain the required result. □

Lemma 3.4. [10] $\mu^1[G] \leq \sqrt{2a - b + 1}$, *where a is size and b is order of a connected graph.*

Lemma 3.5. [11] *Let $M = (m_{i,j})$ and $N = (n_{i,j})$ are two nonnegative symmetric matrices of order a. If $M \geq N$, then $\mu^1[M] \geq \mu^1[N]$.*

Theorem 3.6. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$\mu_{ag}^1[\mathfrak{G}_{\mathcal{P}}] \leq \frac{\alpha}{2\sqrt{\alpha-1}}\sqrt{3\alpha-5-2q(1-2q)}.$$

Proof. Since $g(y) = y + \frac{1}{y}$ is an increasing function on interval $[1, \infty)$, therefore for all edges $w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})$ we have

$$\sqrt{\frac{d_i[\mathfrak{G}_{\mathcal{P}}]}{d_j[\mathfrak{G}_{\mathcal{P}}]}} + \sqrt{\frac{d_j[\mathfrak{G}_{\mathcal{P}}]}{d_i[\mathfrak{G}_{\mathcal{P}}]}} \leq \sqrt{\frac{\alpha-1}{2}} + \sqrt{\frac{2}{\alpha-1}} \leq \frac{\alpha}{\sqrt{\alpha-1}}.$$

Let $\mu^1[\mathfrak{G}_{\mathcal{P}}]$ be a spectral radius of the matrix $\frac{1}{2}\big(\sqrt{\frac{\alpha-1}{2}} + \sqrt{\frac{2}{\alpha-1}}\big)A[\mathfrak{G}_{\mathcal{P}}]$. By Lemmas 3.4 and 3.5, we have

$$\begin{aligned}\mu_{ag}^1[\mathfrak{G}_{\mathcal{P}}] &\leq \frac{1}{2}\big(\sqrt{\frac{\alpha-1}{2}} + \sqrt{\frac{2}{\alpha-1}}\big)\mu^1[\mathfrak{G}_{\mathcal{P}}] \\ &\leq \frac{\alpha}{2\sqrt{\alpha-1}}\sqrt{3\alpha-5-2q(1-2q)}.\end{aligned}$$

□

Lemma 3.7. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$M_1[\mathfrak{G}_{\mathcal{P}}] = 2\alpha^2 + (q+1)(8q^2-6).$$

Proof. Note that by definition

$$M_1[\mathfrak{G}_{\mathcal{P}}] = \sum_{w_iw_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} (d_{w_i}[\mathfrak{G}_{\mathcal{P}}] + d_{w_j}[\mathfrak{G}_{\mathcal{P}}])$$

$$=(2\alpha-2)|E_1[\mathfrak{G}_{\mathcal{P}}]| + (4q+2)|E_2[\mathfrak{G}_{\mathcal{P}}]| + (2q+\alpha)|E_3[\mathfrak{G}_{\mathcal{P}}]| \quad +(\alpha+1)|E_4[\mathfrak{G}_{\mathcal{P}}]|.$$

From Lemmas 2.1 and Proposition 2.2, we have $M_1[\mathfrak{G}_{\mathcal{P}}] = 2\alpha^2 + (q+1)(8q^2-6)$. □

Theorem 3.8. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$\mu_{ag}^1[\mathfrak{G}_{\mathcal{P}}] \geq \frac{2\alpha^2 + (q+1)(8q^2-6)}{(\alpha-1)\alpha}.$$

Proof. Let $Y = (y_1, y_2, ..., y_\alpha)^t$ be a unit vector in $\mathbf{R}^\alpha$. Then

$$
\begin{aligned}
Y^t A_{ag}[\mathfrak{G}_{\mathcal{P}}]Y &= \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} \frac{d_i[\mathfrak{G}_{\mathcal{P}}] + d_j[\mathfrak{G}_{\mathcal{P}}]}{\sqrt{d_i[\mathfrak{G}_{\mathcal{P}}] d_j[\mathfrak{G}_{\mathcal{P}}]}} y_i y_j \\
&\geq \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} \frac{d_j[\mathfrak{G}_{\mathcal{P}}] + d_i[\mathfrak{G}_{\mathcal{P}}]}{\alpha - 1} y_i y_j.
\end{aligned}
$$

Take $Y = \left(\frac{1}{\sqrt{\alpha}}, \frac{1}{\sqrt{\alpha}}, ..., \frac{1}{\sqrt{\alpha}}, \right)^t$. Then from Lemma 3.1, we have

$$
\mu_{ag}^1[\mathfrak{G}_{\mathcal{P}}] \geq Y^t A_{ag}[\mathfrak{G}_{\mathcal{P}}]Y \geq \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} \frac{d_j[\mathfrak{G}_{\mathcal{P}}] + d_i[\mathfrak{G}_{\mathcal{P}}]}{(\alpha - 1)\alpha}.
$$

Now by using Theorem 3.7, we get the required result. □

Lemma 3.9. [3] *Let G be a graph of order a, with degree sequence $d_1, d_2, ..., d_a$, then $\mu^1[G] \geq \sqrt{\frac{M_1[G]}{a}}$.*

Theorem 3.10. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$
\mu_{ag}^1[\mathfrak{G}_{\mathcal{P}}] \geq \sqrt{\frac{2\alpha^2 + (q+1)(8q^2 - 6)}{\alpha}}.
$$

Proof. As

$$
\frac{1}{2}[\sqrt{\frac{d_i[\mathfrak{G}_{\mathcal{P}}]}{d_j[\mathfrak{G}_{\mathcal{P}}]}} + \sqrt{\frac{d_j[\mathfrak{G}_{\mathcal{P}}]}{d_i[\mathfrak{G}_{\mathcal{P}}]}}] \geq 1,
$$

therefore $A_{ag}[\mathfrak{G}_{\mathcal{P}}] \geq A[\mathfrak{G}_{\mathcal{P}}]$. By Lemmas 3.7 and 3.9 we have

$$
\mu_{ag}^1[\mathfrak{G}_{\mathcal{P}}] \geq \sqrt{\frac{\sum_{i=1}^{\alpha} d_i[\mathfrak{G}_{\mathcal{P}}]}{\alpha}} \geq \sqrt{\frac{2\alpha^2 + (q+1)(8q^2 - 6)}{\alpha}}.
$$

□

Lemma 3.11. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$
R_{-\frac{1}{2}}[\mathfrak{G}_{\mathcal{P}}] = \frac{1 + \sqrt{2}\sqrt{\alpha - 1}(\alpha - 2q - 2)}{\alpha - 1} + \frac{2q}{2q+1}\left(\frac{\sqrt{\alpha - 1}(q-1) + 2\sqrt{2q+1}}{\sqrt{\alpha - 1}}\right).
$$

Proof. Note that by definition

$$R_{-\frac{1}{2}}[\mathfrak{G}_{\mathcal{P}}] = \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} \frac{1}{\sqrt{d_{w_i}[\mathfrak{G}_{\mathcal{P}}] d_{w_j}[\mathfrak{G}_{\mathcal{P}}]}}$$

$$= \frac{1}{\sqrt{(\alpha-1)^2}}|E_1[\mathfrak{G}_{\mathcal{P}}]| + \frac{1}{2q+1}|E_2[\mathfrak{G}_{\mathcal{P}}]| + \frac{1}{\sqrt{(2q+1)(\alpha-1)}}|E_3[\mathfrak{G}_{\mathcal{P}}]| + \frac{1}{\sqrt{2(\alpha-1)}}|E_4[\mathfrak{G}_{\mathcal{P}}]|.$$

From Lemma 2.1 and Proposition 2.2, we have

$$R_{-\frac{1}{2}}[\mathfrak{G}_{\mathcal{P}}] = \frac{1}{\alpha-1} + \frac{2q^2-q}{2q+1} + \frac{4q}{\sqrt{(2q+1)(\alpha-1)}} + \frac{\sqrt{2}(e-2)}{\sqrt{\alpha-1}}$$

$$= \frac{1+\sqrt{2}\sqrt{\alpha-1}(\alpha-2q-2)}{\alpha-1} + \frac{2q}{2q+1}\left(\frac{\sqrt{\alpha-1}(q-1)+2\sqrt{2q+1}}{\sqrt{\alpha-1}}\right).$$

□

3.1. On Arithmetic Geometric Energy of Apéry Poset Graphs.

Theorem 3.12. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$Z[\mathfrak{G}_{\mathcal{P}}] = \frac{1}{(\alpha-1)^2} + \frac{q(2q-1)}{(2q+1)^2} + \frac{4q}{(\alpha-1)(2q+1)} + \frac{\alpha-2q-2}{\alpha-1}.$$

Proof. Note that by definition

$$Z[\mathfrak{G}_{\mathcal{P}}] = \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} \frac{1}{d_{w_i}[\mathfrak{G}_{\mathcal{P}}] d_{w_j}[\mathfrak{G}_{\mathcal{P}}]}$$

$$= \frac{1}{(\alpha-1)^2}|E_1[\mathfrak{G}_{\mathcal{P}}]| + \frac{1}{(2q+1)^2}|E_2[\mathfrak{G}_{\mathcal{P}}]| + \frac{1}{(2q+1)(\alpha-1)}|E_3[\mathfrak{G}_{\mathcal{P}}]| + \frac{1}{2(\alpha-1)}|E_4[\mathfrak{G}_{\mathcal{P}}]|.$$

From Table 1 and 2, we have

$$Z[\mathfrak{G}_{\mathcal{P}}] = \frac{1}{(\alpha-1)^2} + \frac{q(2q-1)}{(2q+1)^2} + \frac{4q}{(\alpha-1)(2q+1)} + \frac{\alpha-2q-2}{\alpha-1}.$$

□

Theorem 3.13. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] \leq \sqrt{2\alpha(\alpha-1)^2[\frac{1}{(\alpha-1)^2} + \frac{q(2q-1)}{(2q+1)^2} + \frac{4q}{(\alpha-1)(2q+1)} + \frac{\alpha-2q-2}{\alpha-1}]}.$$

Proof. We know that

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] = \sum_{i=1}^{\alpha} |\mu_{ag}^i|.$$

By the Cauchy Schwarz Inequality,

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] \leq \sqrt{\alpha \sum_{i=1}^{\alpha} (\mu_{ag}^i)^2}$$

$$= \sqrt{\frac{\alpha}{2} \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} (\sqrt{\frac{d_i[\mathfrak{G}_{\mathcal{P}}]}{d_j[\mathfrak{G}_{\mathcal{P}}]}} + \sqrt{\frac{d_j[\mathfrak{G}_{\mathcal{P}}]}{d_i[\mathfrak{G}_{\mathcal{P}}]}})^2}. \tag{3. 1}$$

Since $\sqrt{\frac{d_i[\mathfrak{G}_{\mathcal{P}}]}{d_j[\mathfrak{G}_{\mathcal{P}}]}} + \sqrt{\frac{d_j[\mathfrak{G}_{\mathcal{P}}]}{d_i[\mathfrak{G}_{\mathcal{P}}]}} \leq \sqrt{\frac{\alpha-1}{2}} + \sqrt{\frac{2}{\alpha-1}}$, therefore from equation (3. 1) and by Theorem 3.12, we obtain the required result. □

Lemma 3.14. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$M_2[\mathfrak{G}_{\mathcal{P}}] = 5\alpha^2 + 3q - 4q\alpha - 10q^2 + 9 - 14\alpha + 4q^3 + 8q^4 + 8q^2\alpha.$$

Proof. Note that by definition

$$M_2[\mathfrak{G}_{\mathcal{P}}] = \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} (d_{w_i}[\mathfrak{G}_{\mathcal{P}}] \times d_{w_j}[\mathfrak{G}_{\mathcal{P}}])$$

$$=(\alpha-1)^2|E_1[\mathfrak{G}_{\mathcal{P}}]| + (2q+1)^2|E_2[\mathfrak{G}_{\mathcal{P}}]| + (2q+1)(\alpha-1)|E_3[\mathfrak{G}_{\mathcal{P}}]|$$

$$+ 2(\alpha-1)|E_4[\mathfrak{G}_{\mathcal{P}}]|.$$

From Lemma 2.1 and Proposition 2.2 we have

$$M_2[\mathfrak{G}_{\mathcal{P}}] = 5\alpha^2 + 3q - 4q\alpha - 10q^2 + 9 - 14\alpha + 4q^3 + 8q^4 + 8q^2\alpha.$$

□

Lemma 3.15. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ. Then*

$$F[\mathfrak{G}_{\mathcal{P}}] = 2\alpha^3 - 6\alpha^2 + 14\alpha + 12q^2 + 24q^3 - 14q + 16q^4 - 18.$$

Proof. Note that by definition

$$F[\mathfrak{G}_{\mathcal{P}}] = \sum_{w_i w_j \in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})} ((d_{w_i}[\mathfrak{G}_{\mathcal{P}}])^2 + (d_{w_j}[\mathfrak{G}_{\mathcal{P}}])^2)$$

$$=2(\alpha-1)^2|E_1[\mathfrak{G}_{\mathcal{P}}]| + 2(2q+1)^2|E_2[\mathfrak{G}_{\mathcal{P}}]| + ((2q+1)^2 + (\alpha-1)^2)|E_3[\mathfrak{G}_{\mathcal{P}}]|$$

$$+ (4 + (\alpha-1)^2)|E_4[\mathfrak{G}_{\mathcal{P}}]|.$$

From Lemma 2.1 and Proposition 2.2 we have

$$F[\mathfrak{G}_{\mathcal{P}}] = 2\alpha^3 - 6\alpha^2 + 14\alpha + 12q^2 + 24q^3 - 14q + 16q^4 - 18.$$

□

Theorem 3.16. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ.*

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] \leq \sqrt{\frac{\alpha}{8}(2\alpha^3 + 4\alpha^2 - 14\alpha - 8q^2 + 32q^3 + 32q^4 - 8q - 8q\alpha + 16q^2\alpha)}.$$

Proof. Since $\sqrt{\frac{d_i[\mathfrak{G}_{\mathcal{P}}]}{d_j[\mathfrak{G}_{\mathcal{P}}]}} + \sqrt{\frac{d_j[\mathfrak{G}_{\mathcal{P}}]}{d_i[\mathfrak{G}_{\mathcal{P}}]}} \leq \frac{d_i[\mathfrak{G}_{\mathcal{P}}]+d_j[\mathfrak{G}_{\mathcal{P}}]}{2}$, therefore from equation 3. 1 , from Lemmas 3.14 and 3.15, we obtain the required result. □

Theorem 3.17. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ.*

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] \leq \frac{1}{2}\sqrt{\alpha(\alpha^3 - 3\alpha^2 + 15\alpha + 14q^2 + 12q^3 - 11q + 8q^4 - 21)}.$$

Proof. We know that

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] = \sum_{i=1}^{\alpha} |\mu_{ag}^i|$$

By the Cauchy Schwarz Inequality,

$$\leq \sqrt{\alpha\sum_{i=1}^{\alpha}(\mu_{ag}^{i})^{2}}$$

$$= \sqrt{\frac{\alpha}{2}\sum_{w_iw_j\in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})}(\sqrt{\frac{d_i[\mathfrak{G}_{\mathcal{P}}]}{d_j[\mathfrak{G}_{\mathcal{P}}]}}+\sqrt{\frac{d_j[\mathfrak{G}_{\mathcal{P}}]}{d_i[\mathfrak{G}_{\mathcal{P}}]}})^{2}}$$

$$= \sqrt{\frac{\alpha}{2}\sum_{w_iw_j\in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})}(\sqrt{\frac{d_i[\mathfrak{G}_{\mathcal{P}}]}{d_j[\mathfrak{G}_{\mathcal{P}}]}}+\sqrt{\frac{d_j[\mathfrak{G}_{\mathcal{P}}]}{d_i[\mathfrak{G}_{\mathcal{P}}]}})+\alpha(2\alpha-3-q+2q^{2})}$$

$$\leq \sqrt{\frac{\alpha}{2}\sum_{w_iw_j\in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})}(\frac{d_i[\mathfrak{G}_{\mathcal{P}}]^{2}+d_j[\mathfrak{G}_{\mathcal{P}}]^{2}}{4})+\alpha(2\alpha-3-q+2q^{2})}.$$

Now, by Lemma 3.15 we get the required result. □

Theorem 3.18. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ.*

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] \geq 2\sqrt{\frac{2\alpha^{2}+(q+1)(8q^{2}-6)}{\alpha}}.$$

Proof. From Theorem 3.10, we have

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] = \sum_{i=1}^{\alpha}|\mu_{ag}^{i}| = 2\sum_{i=1,\mu_{ag}^{i}\geq 0}^{\alpha}\mu_{ag}^{i} \geq 2\mu_{ag}^{1} \geq 2\sqrt{\frac{2\alpha^{2}+(q+1)(8q^{2}-6)}{\alpha}}.$$

□

Theorem 3.19. *Let $\mathfrak{G}_{\mathcal{P}}$ be a graph of a poset $\mathcal{P}$ associated with Υ.*

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] \geq 2\sqrt{2\alpha-3-q+2q^{2}}.$$

Proof. Since

$$(E_{ag}[\mathfrak{G}_{\mathcal{P}}])^{2} = \sum_{i=1}^{\alpha}(\mu_{ag}^{i})^{2} + 2\sum_{1\leq i\leq j\alpha}|\mu_{ag}^{i}||\mu_{ag}^{j}|$$

$$\geq \sum_{i=1}^{\alpha}(\mu_{ag}^{i})^{2} + 2\sum_{1\leq i\leq j\alpha}|\mu_{ag}^{i}\mu_{ag}^{j}|$$

$$= 2\sum_{i=1}^{\alpha}(\mu_{ag}^{i})^{2} = \sum_{w_iw_j\in \mathrm{E}(\mathfrak{G}_{\mathcal{P}})}\Big(\frac{d_i[\mathfrak{G}_{\mathcal{P}}]+d_j[\mathfrak{G}_{\mathcal{P}}]}{\sqrt{d_i[\mathfrak{G}_{\mathcal{P}}]d_j[\mathfrak{G}_{\mathcal{P}}]}}\Big)^{2} \geq 4(2\alpha-3-q+2q^{2}),$$

Hence

$$E_{ag}[\mathfrak{G}_{\mathcal{P}}] \geq 2\sqrt{2\alpha-3-q+2q^{2}}.$$

$\square$

Table 3 Numerical Comparison of AG Radius Bounds for $q = 1$

α	q	$\|E(G_P)\|$	Th. 3.10	Th. 3.8	Th. 3.6	$\mu_{ag}^{1}[\mathfrak{G}_{\mathcal{P}}]$
5	1	8	3.286	2.700	4.330	8.163
7	1	12	3.817	2.429	6.062	12.000
9	1	16	4.294	2.306	7.794	15.500
11	1	20	4.729	2.236	9.526	19.000
13	1	24	5.129	2.192	11.258	22.500

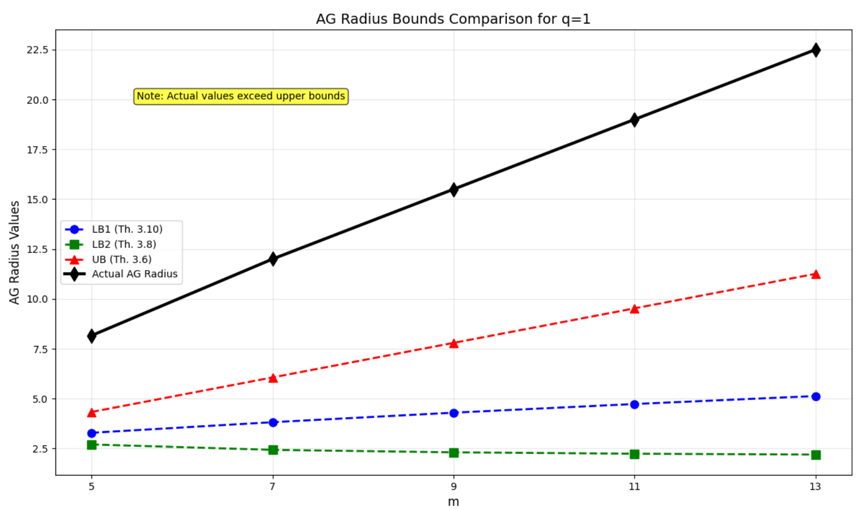
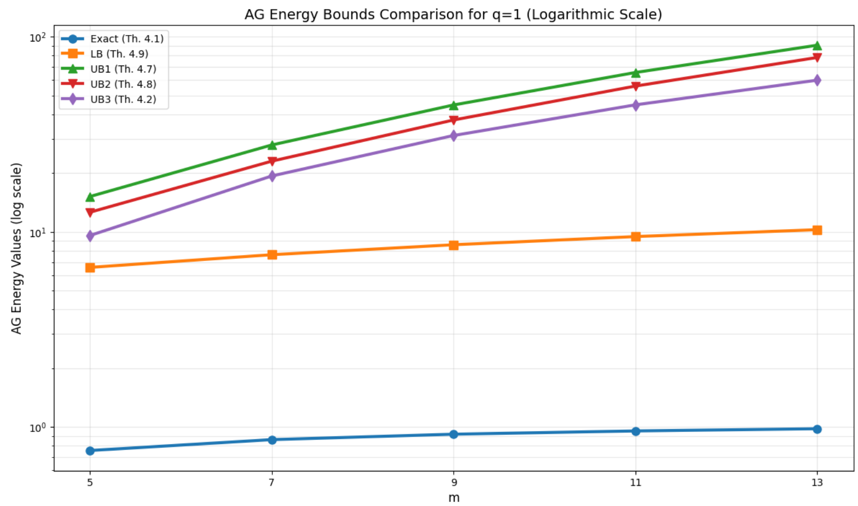


Table 4 Numerical Comparison of AG Energy Bounds for $q = 1$

α	Exact (Th. 3.13)	(Th. 3.16)	(Th. 3.17)	(Th. 3.18)	(Th. 3.19)
5	0.757	6.572	15.166	12.599	9.575
7	0.861	7.634	27.875	23.027	19.332
9	0.918	8.588	44.700	37.440	31.174
11	0.954	9.458	65.582	55.868	44.765
13	0.979	10.258	90.499	78.312	59.909



In the given class of symmetric numerical semigroups, the Apéry poset graphs are never regular, hence the per-edge contributions are not constant. Therefore, none of the bounds of arithmetic geometric spectral radius and arithmetic geometric energy of Graph $\mathfrak{G}_{\mathcal{P}}$ can be sharp.

4. Conclusion

In this research work, we compute different invariants of graphs associated with Apéry poset graphs and give some bounds for the energy and arithmetic geometric radius of Apéry poset graphs in terms of these invariants. In the future, we can extend these investigations to broader classes of numerical semigroups and establish sharper bounds for invariants like the Atom-Bond Connectivity index. Furthermore, the study of additional degree-based indices, such as the Randić, and forgotten indices, may reveal complementary structural information and enhance predictive applications in chemical graph theory. Such developments would not only strengthen the theoretical foundations of Apéry poset graphs but also expand their potential relevance in modeling stability and reactivity in molecular systems. Moreover, we can compute the degree sequences and size of Apéry poset graphs for various types of numerical semigroups, as well as for symmetric numerical semigroups with various embedding dimensions. Additionally, we will use these invariants to illustrate various topological indices.

Credit Authorship Contribution's Statement:

Anam Shahzadi: Conceptualization; Methodology; Formal analysis, Development of examples; Theoretical investigation; Writing – original draft; Visualization; LaTeX preparation and formatting; Primary review and editing.

Muhammad Ahsan Binyamin: Supervision; conceptual guidance; validation of results; critical review and editing of the manuscript; refinement of proofs.

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