Annals of Pure and Applied Mathematics
Vol. 25, No. 1, 2022, 1-5
ISSN: 2279-087X (P), 2279-0888(online)
Published on 11 February 2022
www.researchmathsci.org
DOI: http://dx.doi.org/10.22457/apam.v25n1a01854

Annals of Pure and Applied Mathematics

Geometric-Quadratic and Quadratic-Geometric Indices

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Received 12 January 2022; accepted 10 February 2022

Abstract. Topological indices are applied to measure the chemical characteristics of chemical compounds. In this study, we introduce the geometric-quadratic (GQ) and quadratic-geometric (QG) indices of a graph and compute the exact values of some standard graphs and benzenoid systems.

Keywords: Geometric-arithmetic index, GQ index, QG index, graph, benzenoid system.

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C35

1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. We refer [1], for other undefined notations and terminologies.

A molecular graph is a graph such that its vertices correspond to the atoms and edges to the bonds. Chemical Graph Theory is a branch of mathematical chemistry, which has an important effect on the development of Chemical Sciences. Several topological indices have been considered in Theoretical Chemistry and have found some applications.

The geometric-arithmetic index [2] of a graph G was defined as

$$GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(u)}.$$

This index was studied, for example, in [3, 4, 5, 6, 7, 8, 9].

Motivated by the definition of geometric-arithmetic index of a graph G, we define the geometric-quadratic index as

$$GQ(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_G(u)d_G(v)}}{\sqrt{(d_G(u)^2+d_G(v)^2)/2}}=\sum_{uv\in E(G)}\frac{\sqrt{2d_G(u)d_G(v)}}{\sqrt{d_G(u)^2+d_G(v)^2}}.$$

This equation consists from geometric mean of end vertex degrees of an edge *uv*, $\sqrt{d_G(u)d_G(v)}$ as numerator and quadratic mean of end vertex degrees of the edge *uv*, $\sqrt{(d_G(u)^2+d_G(v)^2)/2}$ as denominator.

Also we introduce the quadratic-geometric index of a graph *G* and defined it as

$$QG(G)=\sum_{uv\in E(G)}\frac{\sqrt{(d_G(u)^2+d_G(v)^2)/2}}{\sqrt{(d_G(u)d_G(v)}}=\sum_{uv\in E(G)}\frac{\sqrt{d_G(u)^2+d_G(v)^2}}{\sqrt{2d_G(u)d_G(v)}}.$$

In this paper, we compute these two newly defined novel graph indices for some standard graphs and benzenoid systems. For benzenoid systems, see [10].

2. Results for some standard graphs

Proposition 1. Let $K_{r,s}$ be a complete bipartite graph with $1 \le r \le$ s, and s $\ge$ 2 vertices. Then

$$GQ(K_{r,s})=\frac{rs\sqrt{2rs}}{\sqrt{r^2+s^2}}.$$

Proof: Let $K_{r,s}$ be a complete bipartite graph with r + s vertices and *rs edges* such that $|V_1|$= r , $|V_2|$= s, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \le r \le$ s, and s $\ge$ 2. Every vertex of V_1 is incident with *s* edges and every vertex of V_2 is incident with r edges.

$$GQ(K_{r,s})=\frac{rs\sqrt{2rs}}{\sqrt{r^2+s^2}}.$$

Corollary 1.1. Let $K_{r,r}$ be a complete bipartite graph with $r \ge 2$. Then

$$GQ(K_{r,r})=r^2.$$

Corollary 1.2. Let $K_{1,r-1}$ be a star with $r \ge 2$. Then

$$GQ(K_{1,r-1})=\frac{(r-1)\sqrt{2(r-1)}}{\sqrt{(r^2-2r+2)}}$$

Proposition 2. If *G* is *r*-regular with *n* vertices and $r \ge 2$, then $GQ(G)=\frac{nr}{2}$.

Proof: Let *G* is *r*-regular with *n* vertices and $r \ge 2$ and $\frac{nr}{2}$ edges. Then

$$GQ(G)=\frac{nr}{2}\frac{\sqrt{2rr}}{\sqrt{(r^2+r^2)}}=\frac{nr}{2}.$$

Corollary 1.1. Let C_n be a cycle with $n \ge 3$ vertices. Then $GQ(C_n)=n.$

Corollary 1.1. Let K_n be a complete graph with $n \ge 3$ vertices. Then

$$GQ(K_n) = \frac{n(n-1)}{2}.$$

Proposition 3. If G is a path with $n \geq 3$ vertices, then

$$GQ(P_n) = n - 3 + \frac{4}{\sqrt{5}}.$$

Proposition 4. Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq$ s, and s ≥ 2 vertices.

Then $$QG(K_{r,s}) = \frac{1}{\sqrt{2}}\sqrt{rs(r^2+s^2)}.$$

Proof: Let $K_{r,s}$ be a complete bipartite graph with $r + s$ vertices and rs *edges* such that $|V_1|=$ r , $|V_2|=$ s, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \leq r \leq$ s, and s ≥ 2. Every vertex of V_1 is incident with s edges and every vertex of V_2 is incident with r edges.

$$QG(K_{r,s}) = \frac{1}{\sqrt{2}}\sqrt{rs(r^2+s^2)}.$$

Corollary 4.1. Let $K_{r,r}$ be a complete bipartite graph with $r \geq 2$. Then $QG(K_{r,r}) = r^2$.

Corollary 4.2. Let $K_{1,r-1}$ be a star with $r \geq 2$. Then

$$QG(K_{1,r-1}) = \frac{1}{\sqrt{2}}\sqrt{(r-1)(r^2-2r+2)}.$$

Proposition 5. If G is r-regular with n vertices and $r \geq 2$, then

$$QG(G) = \frac{nr}{2}.$$

Proof: Let G is r-regular with n vertices and $r \geq 2$ and $\frac{nr}{2}$ edges. Then

$$QG(G) = \frac{nr}{2}\frac{\sqrt{(r^2+r^2)}}{\sqrt{2rr}} = \frac{nr}{2}.$$

Corollary 5.1. Let C_n be a cycle with $n \geq 3$ vertices. Then $QG(C_n) = n$.

Corollary 5.1. Let K_n be a complete graph with $n \geq 3$ vertices. Then

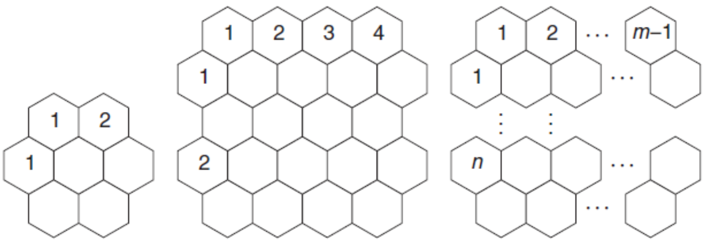
$$QG(K_n) = \frac{n(n-1)}{2}.$$

Proposition 6. If G is a path with $n \geq 3$ vertices, then $QG(P_n) = n - 3 + \sqrt{5}$.

3. Results for Benzenoid Systems

We focus on the chemical graph structure of a jagged rectangle benzenoid system, denoted by $B_{m,n}$ for all m, n, in N. Three chemical graphs of a jagged rectangle benzenoid system are depicted in Figure 1.

Let $H = B_{m,n}$. Clearly the vertices of H are either of degree 2 or 3, see Figure 1. By calculation, we obtain that H has $4mn + 4m + m - 2$ vertices and $6mn + 5m + n - 4$ edges. In H, there are three types of edges based on the degree of end vertices of each edge as given in Table 1.



$B_{3,1}$ $B_{5,2}$ $B_{m,n}$

Figure 1

$d_H(u)\ d_H(v)\backslash uv \in E(H)$	(2,2)	(2,3))	(3, 3)
Number of edges	$2n+4$	$4m+4n-4$	$6mn + m - 5n - 4$

Table 1: Edge partition of $B_{m,n}$

In the following theorem, we determine the Geometric-quadratic index of $B_{m,n}$.

Theorem 1. Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$GQ(B_{m,n}) = 6mn + \left(1 + \frac{8\sqrt{3}}{\sqrt{13}}\right)m + \left(\frac{8\sqrt{3}}{\sqrt{13}} - 3\right)n - \frac{8\sqrt{3}}{\sqrt{13}}.$$

Proof: Let $H = B_{m,n}$. By using equation and Table 1, we deduce

$$GQ(H) = \sum_{uv \in E(H)} \frac{\sqrt{2d_H(u)d_H(v)}}{\sqrt{d_H(u)^2 + d_H(v)^2}}$$

$$= \frac{(2n+4)\sqrt{2\times2\times2}}{\sqrt{2^2+2^2}} + \frac{(4m+4n-4)\sqrt{2\times2\times3}}{\sqrt{2^2+3^2}} + \frac{(6mn+m-5n-4)\sqrt{2\times3\times3}}{\sqrt{3^2+3^2}}.$$

After simplification, we obtain the desired result.

Theorem 2. Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$QG(B_{m,n}) = 6mn + \left(1 + \frac{2\sqrt{13}}{\sqrt{3}}\right)m + \left(\frac{2\sqrt{13}}{\sqrt{3}} - 3\right)n - \frac{2\sqrt{13}}{\sqrt{3}}.$$

Proof: Let $H = B_{m,n}$. By using equation and Table 1, we deduce

$$QG(H) = \sum_{uv \in E(G)} \frac{\sqrt{d_H(u)^2 + d_H(v)^2}}{\sqrt{2d_H(u)d_H(v)}}$$

$$= \frac{(2n+4)\sqrt{2^2+2^2}}{\sqrt{2\times 2\times 2}} + \frac{(4m+4n-4)\sqrt{2^2+3^2}}{\sqrt{2\times 2\times 3}} + \frac{(6mn+m-5n-4)\sqrt{3^2+3^2}}{\sqrt{2\times 3\times 3}}$$

gives the desired result after simplification.

3. Conclusion

In this paper, we have introduced the geometric-quadratic index and quadratic-geometric index of a graph. We have determined exact values of these two novel graph indices for some standard graphs and also for benzenoid systems. Many questions are suggested by this research, among them are the following:

1. Characterize the GQ and QG indices in term of other degree based topological indices.
2. Obtain the extremal values and extremal graphs of GQ and QG indices.
3. Compute the exact values of these two indices for other chemical nanostructures.

Acknowledgement. (1) This work is supported by IGTRC No. BNT/IGRTC/2022:2201:101 International Graph Theory Research Center, Banhatti 587311, India.

(2) The author is thankful to the referee for useful comments.

Conflict of interest. The authors declare that they have no conflict of interest.

Authors' Contributions. All the authors contributed equally to this work.

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