J. Appl. Math. & Informatics Vol. **34***(2016), No. 5 - 6, pp. 479 - 486*
http://dx.doi.org/10.14317/jami.2016.479

EDGE VERSION OF HARMONIC INDEX AND HARMONIC POLYNOMIAL OF SOME CLASSES OF GRAPHS

RABIA NAZIR, SHOAIB SARDAR, SOHAIL ZAFAR* AND ZOHAIB ZAHID

Abstract. In this paper we define the edge version of harmonic index and harmonic polynomial of a graph G. We computed explicit formulas for the edge version of harmonic index and harmonic polynomial of many well known classes of graphs.

AMS Mathematics Subject Classification : 05C07, 05C90.
Key words and phrases : Topological indices, line graph.

1. Introduction and Preliminaries

Let G be a simple graph, with vertex set $V(G)$ and edge set $E(G)$. The degree d_v of a vertex v is the number of vertices joining to v and the degree of an edge $e \in E(G)$, d_e is the number of its adjacent vertices in $V(L(G))$, where $L(G)$ is the line graph of a graph G which is defined as the graph whose vertices are the edges of G, with two vertices are adjacent if the corresponding edges have one vertex common in G.

Line graphs are very useful in structural chemistry, but in recent years they were considered very little in chemical graph theory. In 1981, Bertz introduced the first topological index on the basis of the line graph in [1], when he was working on molecular branching. After that many topological indices based on line graphs were introduced (see [4, 5, 9]). For more details about the applications of line graphs in chemistry, we refer the articles (see [6, 7, 8]).

In chemistry, molecular structure descriptors are used to model information of molecules, which are known as topological indices. They are invariant under graph isomorphisms. There are many topological indices defined on the basis

Received October 15, 2015. Revised January 24, 2016. Accepted January 30, 2016.
*Corresponding author.

of the vertex-degrees of graphs (see [11, 12, 14, 15, 16, 19]). One of the vertex-degree based index namely harmonic index $H(G)$ is first time introduced in [2]:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

For more results on harmonic index we refer to the articles [3, 13, 17, 18, 20, 21, 22, 23]. The harmonic polynomial is defined in [10] as follows

$$H(G,x) = \sum_{uv \in E(G)} 2x^{d_u + d_v - 1}.$$

Note that $\int_0^1 H(G,x)dx = H(G)$.

In a natural way, we introduce the edge version of harmonic index on the basis of the end-vertex degrees of edges in a line graph of G which is defined as:

$$H_e(G) = \sum_{ef \in E(L(G))} \frac{2}{d_e + d_f}.$$

Similarly the edge version of harmonic polynomial is defined as

$$H_e(G,x) = \sum_{ef \in E(L(G))} 2x^{d_e + d_f - 1}.$$

Clearly $\int_0^1 H_e(G,x)dx = H_e(G)$.

The following lemma is helpful for computing the degree of a vertex of line graph.

Lemma 1.1. *Let G be a graph with $u, v \in V(G)$ and $e = uv \in E(G)$. Then:*

$$d_e = d_u + d_v - 2.$$

In order to calculate the number of edges of an arbitrary graph, the following lemma is significant for us.

Lemma 1.2. *Let G be a graph. Then*

$$\sum_{u \in V(G)} d_u = 2|E(G)|.$$

This is also known as handshaking Lemma.

In this paper we computed edge version of harmonic index and harmonic polynomial for the case of regular, complete bipartite, wheel, helm, ladder and $[n]$-pentacene graphs.

2. Main results

Proposition 2.1. *Let G be a k-regular graph of n vertices, then*

(1) $H_e(G,x) = kn(k-1)x^{4k-5}$.
(2) $H(G) = \frac{kn}{4(k-1)}$.

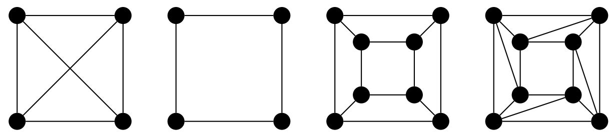

FIGURE 1. The graphs K_n , C_n , π_n and A_n for $n = 4$ from left to right

Proof. Since G is a k- regular graph, then each vertex of G has degree k and by Lemma 1.2 we have $\frac{kn}{2}$ edges. Therefore in $L(G)$ we have $\frac{kn}{2}$ vertices and by using Lemma 1.1, all the vertices have degree $2k-2$. Lemma 1.2 implies that we have $\frac{kn(k-1)}{2}$ edges in $L(G)$. Consequently we get $H_e(G,x) = kn(k-1)x^{4k-5}$. □

Let K_n, C_n, Π_n and A_n denotes the complete graph on n vertices, the cycle on n vertices, the n-sided prism and the n-sided antiprism as shown in Fig. 1.

Proposition 2.2. *We have*

(1) $H_e(K_n, x) = n(n-1)(n-2)x^{4n-9}$ *and* $H_e(K_n) = \frac{n(n-1)}{4}$.
(2) $H_e(C_n, x) = 2nx^3$ *and* $H_e(C_n) = \frac{n}{2}$.
(3) $H_e(\Pi_n, x) = 12nx^{11}$ *and* $H_e(\Pi_n) = n$.
(4) $H_e(A_n, x) = 30nx^{19}$ *and* $H_e(A_n) = \frac{3n}{2}$.

Proof. This proof can be obtained by using Proposition 2.1. □

.

Proposition 2.3. *Let G be a complete bipartite graph $K_{m,n}$ of $m+n$ vertices and mn edges, then*

(1) $H_e(k_{m,n}, x) = mn(m+n-2)x^{2m+2n-5}$.
(2) $H_e(k_{m,n}) = \frac{mn}{2}$.

Proof. In G there are m vertices of degree n and remaining n vertices of degree m. In $L(G)$ there are mn vertices and each vertex have degree $m+n-2$ by Lemma 1.1. By Lemma 1.2, $L(G)$ has $mn(\frac{m+n-2}{2})$ edges. Consequently we get $H_e(k_{m,n}, x) = mn(m+n-2)x^{2m+2n-5}$and $H_e(k_{m,n}) = \frac{mn}{2}$. □

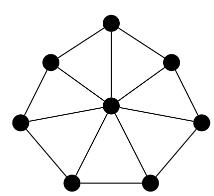

FIGURE 2. The wheel graph W_7

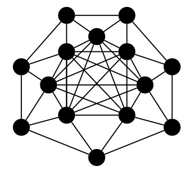

FIGURE 3. The line graph of wheel graph W_7

Proposition 2.4. *Let W_n be a graph of wheel, then*

(1) $H_e(W_n, x) = 2nx^7 + n(n-1)x^{2n+1} + 4nx^{n+4}$.
(2) $H_e(W_n) = \frac{n}{4} + \frac{n(n-1)}{2(n+1)} + \frac{4n}{n+5}$.

Proof. In the wheel graph W_n, the total number of vertices and edges are $n+1$ and $2n$ respectively (see Fig. 2). Therefore in $L(W_n)$, the total number of vertices are $2n$, out of which n vertices of degree 4 and remaining n vertices of degree $n+1$ (see Fig. 3). It is easily seen from Lemma 1.2 that the total number of edges in $L(W_n)$ are $\frac{n(n+5)}{2}$. The edge partition of $E(L(W_n))$ based on the degree of the vertices is shown in Table 1.

TABLE 1. The edge partition of $L(W_n)$

(d_e, d_f)	$(4, 4)$	$(n+1, n+1)$	$(4, n+1)$
Number of edges	n	$\frac{n(n-1)}{2}$	$2n$

Hence we get $H_e(W_n, x) = 2nx^7 + n(n-1)x^{2n+1} + 4nx^{n+4}$ and $H_e(W_n) = \frac{n}{4} + \frac{n(n-1)}{2(n+1)} + \frac{4n}{n+5}$. □

Proposition 2.5. *Let H_n be a helm graph, then*

(1) $H_e(H_n, x) = 4nx^8 + 4nx^{n+7} + n(n-1)x^{2n+3} + 2nx^{n+4} + 2nx^{11}$.
(2) $H_e(H_n) = \frac{4n}{9} + \frac{4n}{n+8} + \frac{n(n-1)}{2(n+2)} + \frac{2n}{n+5} + \frac{n}{n+6}$.

Proof. In the helm graph H_n, the total number of vertices and edges are $2n+1$ and $3n$ respectively (see Fig. 4). Therefore in $L(H_n)$, the total number of vertices are $3n$, out of which n vertices of degree 3, n vertices of degree 6 and n vertices of degree $n+2$ (see Fig. 5). It is easily seen from Lemma 1.2 that the total number of edges in $L(H_n)$ are $\frac{n(n+11)}{2}$. The edge partition of $E(L(H_n))$ based on the degree of the vertices is shown in Table 2.

TABLE 2. The edge partition of $L(H_n)$

(d_e, d_f)	$(3, 6)$	$(6, n+2)$	$(n+2, n+2)$	$(3, n+2)$	$(6, 6)$
Number of edges	$2n$	$2n$	$\frac{n(n-1)}{2}$	n	n

Therefore we get $H_e(H_n, x) = 4nx^8 + 4nx^{n+7} + n(n-1)x^{2n+3} + 2nx^{n+4} + 2nx^{11}$ and $H_e(H_n) = \frac{4n}{9} + \frac{4n}{n+8} + \frac{n(n-1)}{2(n+2)} + \frac{2n}{n+5} + \frac{n}{6}$. □

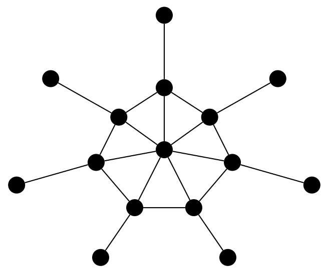

FIGURE 4. The helm graph H_7

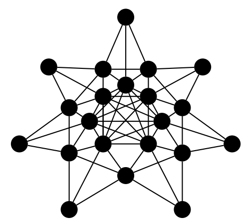

FIGURE 5. The line graph of helm graph H_7

Proposition 2.6. *Let L_n be a graph of ladder, then*

(1)

$$H_e(L_n, x) = \begin{cases} 8x^4 + 16x^6 + 2(6n-14)x^7, & \textit{if} \quad n > 2 \ ; \\ 8x^4 + 4x^5 + 8x^6, & \textit{if} \quad n = 2 \ . \end{cases}$$

(2)

$$H_e(L_n) = \begin{cases} \frac{105n+517}{70}, & \textit{if} \quad n > 2 \ ; \\ \frac{358}{105}, & \textit{if} \quad n = 2 \ . \end{cases}$$

Proof. The ladder graph L_n for $n = 1$ is a cycle C_4 which is known from Proposition 2.1. For L_2 we have the edge partition of $E(L(L_2))$ based on the degree of the vertices is shown in Table 3.

TABLE 3. The edge partition of $L(L_2)$

(d_e, d_f)	$(2,3)$	$(3,3)$	$(3,4)$
Number of edges	4	2	4

In the ladder graph L_n for $n > 2$, the total number of vertices and edges are $2n+2$ and $3n+1$ respectively (see Fig. 6). Therefore in $L(L_n)$, the total number of vertices are $3n + 1$, out of which 2 vertices of degree 2, 4 vertices of degree 3 and $3n - 5$ vertices of degree 4 (see Fig. 7). It is easily seen from Lemma 1.2 that the total number of edges in $L(L_n)$ are $6n - 2$. The edge partition of

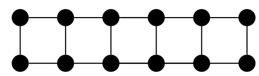

FIGURE 6. The ladder graph L_5

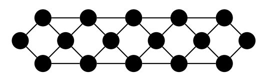

FIGURE 7. The line graph of ladder graph L_5

$E(L(L_n))$ based on the degree of the vertices is shown in Table 4.

TABLE 4. The edge partition of $L(L_n)$

(d_e, d_f)	$(2,3)$	$(3,4)$	$(4,4)$
Number of edges	4	8	$6n-14$

Consequently, we get $H_e(L_n, x) = 8x^4 + 16x^6 + 2x^7(6n-14)$ and $H_e(L_n) = \frac{105n+517}{70}$. □

In chemistry, the pentacene compound is a hydrocarbon consists of five benzene rings. It is purple powder organic semiconductor and gradually degrades when exposed to light and air. The linear $[n]$-Pentacene P_n for $n = 2$ is shown in Fig. 8.

Proposition 2.7. *Let P_n be a graph of linear $[n]$-pentacene, then*
(1) $H_e(P_n, x) = 8x^3 + 8x^4 + (36n-8)x^5 + (48n-16)x^6 + (8n-8)x^7$).
(2) $H_e(P_n) = \frac{97n}{7} - \frac{107}{105}$.

Proof. In the pentacene graph P_n the total number of vertices and edges are $22n$ and $28n-2$ respectively (see Fig. 8). Therefore in line graph $L(P_n)$, the total number of vertices are $28n-2$ out of which 6 vertices are of degree 2, $20n-4$ vertices are of degree 3 and $8n-4$ vertices are of degree 4 (see Fig. 9). It is easily seen from Lemma 1.2 that the total number of edges in $L(P_n)$ are $46n-8$. The edge partition of $E(L(P_n))$ based on the degree of the vertices in shown in Table 5.

TABLE 5. The edge partition of $L(P_n)$

(d_e, d_f)	$(2,2)$	$(2,3)$	$(3,3)$	$(3,4)$	$(4,4)$
Number of edges	4	4	$18n-4$	$24n-8$	$4(n-1)$

Hence we get $H_e(P_n, x) = 8x^3 + 8x^4 + (36n-8)x^5 + (48n-16)x^6 + (8n-8)x^7$ and $H_e(P_n) = \frac{97n}{7} - \frac{107}{105}$. □

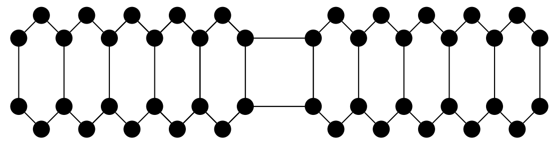

FIGURE 8. The pentacene graph P_2

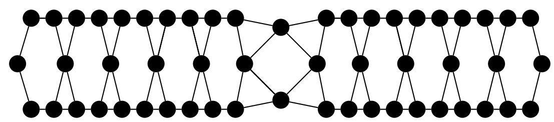

FIGURE 9. The line graph of pentacene P_2

REFERENCES

1. S.H. Bertz, *The bond graph*, J.C.S. Chem. Commun. 1981, 818-820.
2. S. Fajtlowicz, *On conjectures of Grafiti II*, Congr. Numer. **60** (1987), 187-197.
3. O. Favaron, M. Maheo and J.F. Sacle, *Some eigenvalue properties in graphs (conjectures of Grafiti II)*, Discrete Math. **111** (1993), 197-220.
4. I. Gutman, *Edge versions of topological indices, in: I. Gutman and B. Furtula (Eds.), Novel Molecular Structure Descriptors - Theory and Applications II* , Univ. Kragujevac **3** (2010).
5. I. Gutman and E. Estrada, *Topological indices based on the line graph of the molecular graph*, J. Chem. Inf. Comput. Sci. **36** (1996), 541-543.
6. I. Gutman, L. Popovic, B. K. Mishra, M. Kaunar, E. Estrada and N. Guevara, *Application of line graphs in physical chemistry. Predicting surface tension of alkanes*, J. Serb. Chem. Soc. **62** (1997), 1025-1029.
7. I. Gutman and Z. Tomovic, *On the application of line graphs in quantitative structure-property studies*, J. Serb. Chem. Soc. **65** (2000), 577-580.
8. I. Gutman and Z. Tomovic, *Modeling boiling points of cycloalkanes by means of iterated line graph sequences*, J. Chem. Inf. Comput. Sci. **41** (2001), 1041-1045.
9. A. Iranmanesh, I. Gutman, O. Khormali and A. Mahmiani, *The edge versions of the Wiener index*, MATCH Comm. Math. Comput. Chem. **61** (2009), 663-672.
10. M.A. Iranmanesh and M. Saheli, *On the harmonic index and harmonic polynomial of Caterpillars with diameter four*, Iranian J. of Math. Chem. **6** (2015), 41-49.
11. X. Li and Y. Shi, *A survey on the Randic?index*, MATCH Commun. Math. Comput. Chem. **59** (2008), 127-156.
12. X. Li, Y. Shi and L. Wang, *An updated survey on the Randic?index*, in: B.F. I. Gutman (Ed.), Recent Results in the Theory of Randic Index, University of Kragujevac and Faculty of Science Kragujevac (2008), 9-47.
13. V. Lokesha, A. Usha, P.S. Ranjini and T. Deepika, *Harmonic Index of Cubic Polyhedral Graphs Using Bridge Graphs*, Applied Mathematical Sciences **85** (2015), 4245-4253.
14. M.F. Nadeem, S. Zafar and Z. Zahid, *Certain topological indicies of the line graph of subdivsion graphs*, Appl. Math. Comput. **271** (2015), 790-794.
15. M.F. Nadeem, S. Zafar and Z. Zahid, *On Topological properties of the line graph of subdivision graphs of certain nanostructures*, Appl. Math. Comput. **273** (2016), 125-130.

16. J. Rada and R. Cruz, *Vertex-degree-based topological indices over graphs*, MATCH Commun. Math. Comput. Chem. **72** (2014), 603-616.
17. P.S. Ranjini, V. Lokesha and A. Usha, *Relation between Phenylene and Hexagonal Squeeze using Harmonic Index*, International Journal of Graph Theory **1** (2013), 116-121.
18. B. Shwetha Shetty, V. Lokesha and P.S. Ranjini, *On the Harmonic Index of Graph Operations*, Transactions on Combinatorics **4** (2015), 5-14.
19. G. Yu and L. Feng, *On connective eccentricity index of graphs*, MATCH Commun. Math. Comput. Chem. **69** (2013), 611-628.
20. X. Xu, *Relationships between harmonic index and other topological indices*, Appl. Math. Sci. **6** (2012), 2013-2018.
21. L. Zhong, *The harmonic index for graphs*, Appl. Math. Lett. **25** (2012), 561-566.
22. L. Zhong, *The harmonic index on unicyclic graphs*, Ars Combin. **104** (2012), 261-269.
23. L. Zhong and K. Xu, *The harmonic index for bicyclic graphs*, Utilitas Math. **90** (2013), 23-32.

Rabia Nazir is student of MS Mathematics at University of Management and Technology (UMT), Lahore Pakistan. Her research interests include graph theory.

Department of Mathematics, University of Management and Technology (UMT), Lahore Pakistan.
e-mail: rabianazir006@gmail.com

Shoaib Sardar is student of MS Mathematics at University of Management and Technology (UMT), Lahore Pakistan. His research interests are computational mathematics and graph theory.

Department of Mathematics, University of Management and Technology (UMT), Lahore Pakistan.
e-mail: shoaibsardar093@gmail.com

Sohail Zafar received Ph.D. from Abdus Salam school of Mathematical sciences, Lahore, Pakistan in 2013, since then he is working as an assistant professor at University of Management and Technology (UMT), Lahore Pakistan. His research interests are computational algebra, graph theory and cryptography.

Department of Mathematics, University of Management and Technology (UMT), Lahore Pakistan.
e-mail: sohailahmad04@gmail.com

Zohaib Zahid received Ph.D. from Abdus Salam school of Mathematical sciences, Lahore, Pakistan in 2014, since then he is working as an assistant professor at University of Management and Technology (UMT), Lahore Pakistan. His research interests are computational algebra and chemical graph theory.

Department of Mathematics, University of Management and Technology (UMT), Lahore Pakistan.
e-mail: zohaib_zahid@hotmail.com