



Research article

Laplacian and signless laplacian spectra and energies of multi-step wheels

Zheng-Qing Chu¹, Mobeen Munir^{2,*}, Amina Yousaf², Muhammad Imran Qureshi³ and Jia-Bao Liu⁴

¹ Department of Mathematics and Physics, Anhui Xinhua University, Hefei 230088, China

² Division of Science and Technology, University of Education, Lahore 54000, Pakistan

³ Department of Mathematics, COMSATS University Islamabad, Vehari campus, Vehari 61100, Pakistan

⁴ School of Mathematics and Physics, Anhui Jianzhu University, Hefei 230601, China

* **Correspondence:** Tel: +92-320-947-2635; Email: mmunir@ue.edu.pk.

Abstract: Energies and spectrum of graphs associated to different linear operators play a significant role in molecular chemistry, polymerisation, pharmacy, computer networking and communication systems. In current article, we compute closed forms of signless Laplacian and Laplacian spectra and energies of multi-step wheel networks $W_{n,m}$. These wheel networks are useful in networking and communication, as every node is one hop neighbour to other. We also present our results for wheel graphs as particular cases. In the end, correlation of these energies on the involved parameters $m \geq 3$ and n is given graphically. Present results are the natural generalizations of the already available results in the literature.

Keywords: laplacian matrix; signless laplacian matrix; spectrum; laplacian energy; signless laplacian energy; wheel graphs

1. Introduction

Graph theory is instrumental in providing the most diversified applications in almost all phenomenons and disciplines. One of the major areas, that connects graph theory with physical and computer sciences is the use of characteristic polynomial, which plays a comprehensive role in quantum chemistry, physical chemistry, molecular topology, networking and communication systems [1–3]. Mathematicians are playing their part in this joint ventures due to the fascinating problems, that take birth because of involment of the discrete geometrical structures. The roots of this polynomial are called eigenvalues corresponding to some particular directions called eigenvectors. Applications of eigenvalues and eigenvectors are perhaps countless. For example, in quantum

mechanics, eigen-state and wave-function are often used interchangeably. Eigenvalue actually represents the value of a measurable quantity associated with the wave-function. As an example, when computing the eigen-states of the Hamiltonian H , the associated eigenvalues represent energies and within the context of the momentum operators, the associated eigen-states refer to the momentum of the particle. Other well-known application is the Schrodinger equation in which each energy level is associated to an energy eigenvalue [4, 5]. Generally speaking, many chemical processes can be modeled as a system of first-order differential equations. The associated homogeneous part has solution space with eigenvalues of the linear operators of associated matrices, which represents solution to that chemical process. In architecture and mechanical engineering, stability is a classic application of eigenvalue analysis. It is also well-known that principal directions and principal curvatures are the eigenvalues of the classical Weingarten map of surfaces and measure the maximum and minimum normal sectional curvature of any surface.

Other application of eigenvalues can be given in image compression, where it is done by throwing away the small eigenvalues of AA^T . Clustering has dynamic role in data analysis in modern age, whether it is in medical imaging, biology and plants, marketing and business or connection amongst fields on facebook. It provides subsystems inside huge data sets [1, 2]. Spectral clustering is important such method, which uses the eigenvalues of graph associated to the given network.

The largest eigenvector of the graph of the internet gives the information that, how the pages are ranked [3]. In the same way, Netflix predicts the rating of the movies. This is what most of the websites operate, [1–3].

Energy of a graph is defined as sum of the absolute values of eigenvalues [6] by Gutman et al.. But the main inspiration for his definition had a long history linking with popular "Huckel Molecular Orbital Theory", [7–9]. New theoretical ideas relating to different energies keep on emerging on the scene. Adjacency energy of a graph which is the sum of the absolute values of the eigenvalues of its adjacency matrix is related to the total π -electron energy of conjugated hydro-carbon molecules. In recent times more than twenty different energies have been introduced, based on eigenvalues of different matrices associated to graphs, [10–13].

Laplacian energy was introduced by Gutman et al., [14, 15] in 2006. Eigenvalues and eigenvectors of the Laplacian matrix are useful in clustering of data. In a network, two largest clusters can be found using the Laplacian Matrix. The eigenvector corresponding to second smallest eigenvalue helps in this regard [1–3]. Results about distance energies have been given in [16, 17]. Some energies are derived by Nikiforov in [18] for non-regular graphs. Authors computed signless Laplacian energies in [19] for some finite graphs.

We compute the formulas for Laplacian and signless Laplacian energies of a multi-step wheel network and then by specialising our results we derive the closed forms of these energies for classical wheel graph. These graphs are particularly important in communication systems. One of the most attractive features of this graph is its one-hop neighborhood, including vertices and edges. This feature makes this graph more reliable and self-stable as communication system [20, 21]. So it is desirable to formulate analytical closed expressions for the different spectra and energies of this graph. This graph can be considered as molecular graph of some molecular chains where vertices are representatives of atoms and edges are the bonds between them. In this sense different energies and different eigen values present potential applications relating to properties of these molecular compounds.

2. Preliminaries

In this section, we put together main ideas and preliminary notions. Let $G = (V, E)$ be a simple connected graph with edge set $E(G)$ and vertex set $V(G)$. Number of vertices and number of edges are called order and size of graph respectively. Number of vertices adjacent to a vertex v is called degree of v and denoted as dv . The Laplacian matrix $L_{n \times n}$, [14, 17] of G of order n is

$$L = D - A$$

where D and A are degree and adjacency matrices of G . Defined as

$$D = [d_{ij}] = \begin{cases} dv_i, & i = j; \\ 0, & \text{otherwise} \end{cases}$$

and

$$A = [a_{ij}] = \begin{cases} 1 & \{v_i, v_j\} \in E(G) \\ 0 & \text{otherwise} \end{cases}$$

From definition it is clear that

$$[L_{ij}] = \begin{cases} dv_i, & i = j; \\ -1, & i \neq j \text{ and } v_i \text{ and } v_j \text{ are adjacent;} \\ 0, & \text{otherwise} \end{cases}$$

The signless Laplacian matrix $Q_{n \times n}$ [19] associated to G of order n is

$$Q = D + A$$

In most of the cases, associated matrices are symmetric and real so eigenvalues are necessarily real. The set consisting of all eigenvalues forms the spectrum of G . The trace is the sum of all eigenvalues. If a graph G is not regular, then its Laplacian and signless Laplacian energies are defined as

$$LE(G) = \sum_{i=1}^n \left| \lambda_i - \frac{2m}{n} \right| \quad (2.1)$$

where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of L . Here m is size of G .

$$QE(G) = \sum_{i=1}^n \left| P_i - \frac{2m}{n} \right| \quad (2.2)$$

where P_1, \dots, P_n are the eigenvalues of Q . In [18], author computed some matrices and energies of graphs. Recently in [22], authors computed distance and incidence energies of classical wheels and generalized wheels. Jia-bao et al. computed incidence energies and asymptotic Laplacian of some lattices in [23, 24]. It makes sense to ask for the other popular closed forms of energies and spectra of this graph. These different forms of energies and spectra of this graphs have potential applications in network, chemistry, molecular topology, physics and other areas.

3. Generalized wheel networks

A generalized or multi-step wheel network, $W_{n,m}$, is a graph derived from m copies of cycles C_n and one vertex v , in such a way that all vertices of each C_n are adjacent to v . Thus order of $W_{n,m}$ is $nm + 1$. The main hub vertex is called center and other vertices are called n -rim vertices. The diameter of this graph is 2 and can be seen easily as the maximum distance between any two vertices. Figure 1 presents an instance of the wheel graph $W_{12,m}$ having M levels.

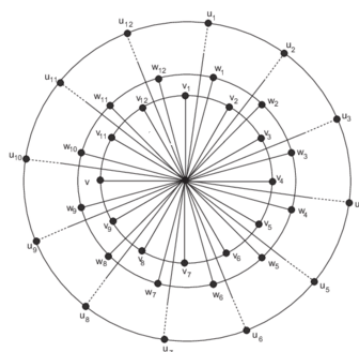


Figure 1. An m -level wheel $W_{12,m}$.

Vertices situated at the same cycle C_n are called rim vertices. This graph is a natural generalization of classical wheel graph W_n . Figure 2 is an example of wheel graph W_6 .

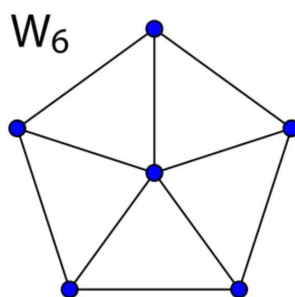


Figure 2. W_6 .

In vulnerability of networks and wireless sensor networks, the wheel graph is being used, see [20, 21]. Jia-Bao et al. computed closed formulas of adjacency and distance energies of these graphs [22]. The wheel graph has many good properties such as the every other vertex is adjacent to the central or hub vertex. Many mathematicians studied different properties of wheel graphs. For comprehensive overview see [20, 25–27]. In this article we are interested to compute closed forms of Laplacian and signless Laplacian energies and spectra of this graph. We also want to obtain these results for classical wheels as special cases of our newly obtained results.

4. Main results

In this section, some results on Laplacian, and signless Laplacian energies are given for wheel related graphs $W_{n,m}$.

Theorem 4.1 The Laplacian energy of wheel graph $W_{n,m}$ is

$$LE(W_{n,m}) = 4mn \quad (4.1)$$

Proof. Let A denotes the adjacency matrix of C_m , given as

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & . & . & . & 0 & 1 \\ 1 & 0 & 1 & 0 & . & . & . & 0 & 0 \\ 0 & 1 & 0 & 1 & . & . & . & 0 & 0 \\ 0 & 0 & 1 & 0 & . & . & . & 0 & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 1 \\ 1 & 0 & 0 & 0 & . & . & . & 1 & 0 \end{pmatrix}$$

where $a_{ij} = 1$ whenever $|i - j| = 1$ or $m - 1$ and all $a_{ij} = 0$ otherwise.

The m -cycles has adjacency spectrum

$$Spec(C_m) = 2 \cos\left(\frac{2\pi j}{m}\right) \text{ where } j = 0, 1, \dots, m-1$$

So the Laplacian matrix of $W_{n,m}$ in the block matrix form is

$$L_{m \times m} = \begin{pmatrix} mn & J_{1 \times m} & J_{1 \times m} & . & . & . & J_{1 \times m} \\ J_{m \times 1} & [G]_{m \times m} & [0]_{m \times m} & . & . & . & [0]_{m \times m} \\ J_{m \times 1} & [0]_{m \times m} & [G]_{m \times m} & . & . & . & [0]_{m \times m} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ J_{m \times 1} & [0]_{m \times m} & [0]_{m \times m} & . & . & . & [0]_{m \times m} \\ J_{m \times 1} & [0]_{m \times m} & [0]_{m \times m} & . & . & . & [G]_{m \times m} \end{pmatrix}$$

where

$$J_{1 \times m} = \begin{pmatrix} 1 & 1 & . & . & . & 1 \end{pmatrix}$$

$$G_{m \times m} = \begin{pmatrix} 3 & -1 & 0 & . & . & . & -1 \\ -1 & 3 & -1 & . & . & . & 0 \\ 0 & -1 & 3 & . & . & . & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & . & -1 \\ -1 & 0 & 0 & . & . & . & 3 \end{pmatrix}$$

By using binomial series, we get the Laplacian spectrum of $W_{n,m}$ as

$$Spec_L(W_{n,m}) = \left(\begin{array}{cccc} 0 & 1 & mn+1 & -\lambda_i+3 \\ 1 & n-1 & 1 & n \end{array} \right) i = 2, \dots, m$$

where λ_i are the eigenvalues of A .

Since $\lambda_i > 0$ for all $i = 2, 3, \dots, p$. Now by using definition, we have $LE(Wn, m) = 4mn$. \square

Theorem 4.2 The signless Laplacian energy of $W_{n,m}$ is given by

$$QE(G)(W_{n,m}) = 3mn - 5 + \sqrt{(mn)^2 - 6mn + 25} \quad (4.2)$$

Proof. Since adjacency matrix of cycle graph is

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & 1 & \dots & 0 & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix}$$

where $a_{ij} = 1$ whenever $|i - j| = 1$ or $m - 1$ and all $a_{ij} = 0$ otherwise.

Since

$$Spec(C_m) = 2 \cos\left(\frac{2\pi j}{m}\right) \text{ where } j = 0, 1, 2, \dots, n-1$$

Then the signless Laplacian matrix of $W_{n,m}$ is

$$Q_{m \times m} = \begin{pmatrix} mn & J_{1 \times m} & J_{1 \times m} & \dots & J_{1 \times m} \\ J_{m \times 1} & [H]_{m \times m} & [0]_{m \times m} & \dots & [0]_{m \times m} \\ J_{m \times 1} & [0]_{m \times m} & [H]_{m \times m} & \dots & [0]_{m \times m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ J_{m \times 1} & [0]_{m \times m} & [0]_{m \times m} & \dots & [0]_{m \times m} \\ J_{m \times 1} & [0]_{m \times m} & [0]_{m \times m} & \dots & [H]_{m \times m} \end{pmatrix}$$

where

$$J_{1 \times m} = \begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix}$$

and

$$H_{m \times m} = \begin{pmatrix} 3 & 1 & 0 & \cdot & \cdot & \cdot & 1 \\ 1 & 3 & 1 & \cdot & \cdot & \cdot & 0 \\ 0 & 1 & 3 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & 1 \\ 1 & 0 & 0 & \cdot & \cdot & \cdot & 3 \end{pmatrix}$$

We get the signless Laplacian spectrum of $W_{n,m}$ by using binomial series and adjacency spectrum of a cycle graph.

$$\text{spec}_Q(W_{n,m}) = \left(\begin{matrix} mn + 5 \pm \frac{1}{2} \sqrt{(mn)^2 - 6mn + 25} & 5 & \lambda_i + 3 \\ 1 & n-1 & n \end{matrix} \right) i = 2, 3, \dots, m$$

where λ_i are the eigenvalues of A .

Since all $\lambda_i > 0$, Now by using definition, we arrive at the desired result of signless Laplacian energy

$$QE(G)(W_{n,m}) = 3mn - 5 + \sqrt{(mn)^2 - 6mn + 25}.$$

Now we derive the particular cases for classical wheel graph. □

Theorem 4.3 Laplacian energy of wheel graph $W_{1,m}$ is

$$LE(W_{1,m}) = 4m. \quad (4.3)$$

Proof. The generalized wheels for $n = 1$ becomes classical wheel graph. Then reiterating the first result we arrive at the desired result. □

Theorem 4.4 Signless Laplacian energy of $W_{1,m}$ is

$$QE(G)(W_{1,m}) = 3m - 5 + \sqrt{m^2 - 6m + 25} \quad (4.4)$$

Proof. The generalized wheels for $n = 1$ becomes classical wheel graph. Then reiterating the second result we arrive at the desired result. □

5. Conclusions and analysis

The present article has been devoted to computation of general forms of Laplacian and signless Laplacian energies of multi-level wheels. These networks are used for communication in networks and mathematical modeling of different chemical structures. We have computed closed analytical expressions of Laplacian and signless Laplacian energies of these graphs which have applications in different areas of networking and molecular topology. keeping the notations intact we obtained the following results,

Theorem The Laplacian energy of $W_{n,m}$ is

$$LE(W_{n,m}) = 4mn \quad (5.1)$$

Theorem The signless Laplacian energy of $W_{n,m}$ is given by

$$QE(G)(W_{n,m}) = 3mn - 5 + \sqrt{(mn)^2 - 6mn + 25} \quad (5.2)$$

Theorem Laplacian energy of $W_{1,m}$ is

$$LE(W_{1,m}) = 4m. \quad (5.3)$$

Theorem Signless Laplacian energy of $W_{1,m}$ is

$$QE(G)(W_{1,m}) = 3m - 5 + \sqrt{m^2 - 6m + 25} \quad (5.4)$$

Our next attempt is the study of behavior of calculated energies on the number of rim vertices and steps of the generalized wheels. Results clearly indicate that two parameters m and n are important for us. We want to correlate these energies with these parameters. We use maple to draw two dimension surfaces for the energies of graphs. Keeping on of the parameter m and n constant, we can easily trace how the energies behave. In the next figures, dependencies of LE on the parameters m and n are given. Results clearly indicate that Laplacian energies rise with increase in both of these parameters.

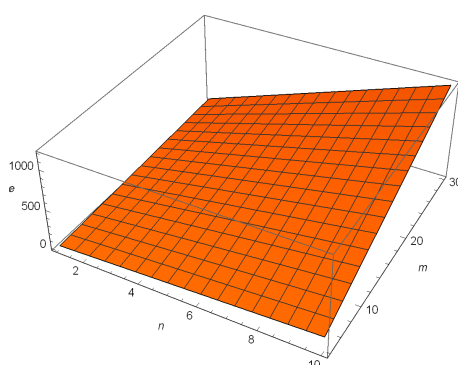


Figure 3. View of Laplacian energy of $W_{n,m}$.

The above surface shows the dependence of Laplacian energy on m and n .

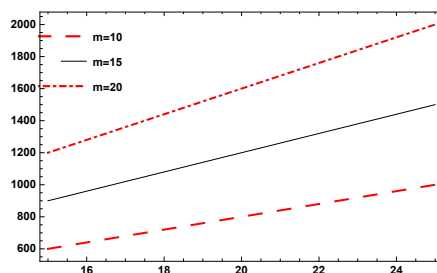


Figure 4. Laplacian energy of $W_{n,m}$ while keeping m constant.

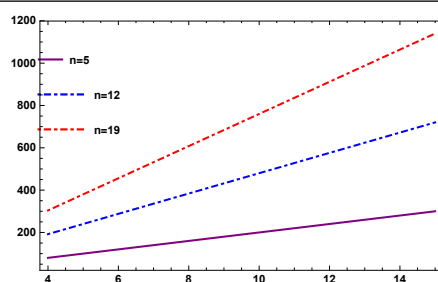


Figure 5. Laplacian energy of $W_{n,m}$ while keeping n constant.

In the next figures, dependencies of QE on the parameters m and n are given. Clearly signless Laplacian energy rises with rise in both of the parameters.

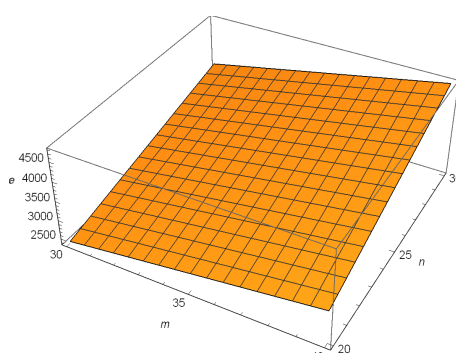


Figure 6. View of QE of $W_{n,m}$.

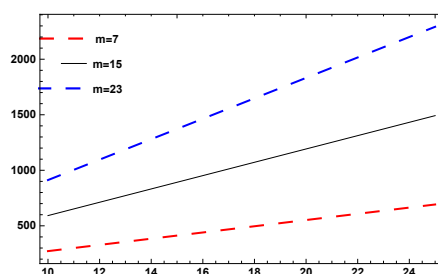


Figure 7. QE of $W_{n,m}$ while keeping m constant.

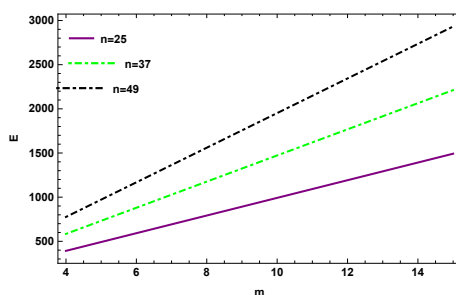


Figure 8. QE of $W_{n,m}$ while keeping n constant.

In this paper, we computed closed forms of Laplacian and signless Laplacian energies of generalized wheels and classical wheel. Since generalized wheel is important cyclic structure having common hub, so our results are helpful for the chemists working in industry. The pictorial dependence of different energies on the involved parameters are presented in an easy understandable way. It is important to remark that by removing some spokes of the wheel graphs we obtain a new wheel graph with lesser number m and n so closed formulas are still applicable.

Acknowledgement

We are thankful to the respected reviewers for the valuable comments which helped us to improve the manuscript. Funding: The authors would like to express their sincere gratitude to the Natural Science Foundation for the Higher Education Institutions of Anhui Province of China (No. KJ2019A0875 and No. KJ2019A0876);

Author contributions

Conceptualization is done by Mobeen Munir, Methodology is developed by Zheng-Qing Chu and Jia-Bao Liu, Writing the original draft is carried out by Amina Yousaf and Muhammad Imran Qureshi.

Conflicts of interest

The authors declare no conflict of interest.

References

1. S. Wang, A. Gittens, M. W. Mahoney, Scalable kernel K-Means clustering with nystrom approximation: Relative-Error bounds, *J. Mach. Learn. Res.*, **20** (2019), 1–49.
2. E. A. Castro, G. Chen, G. Lerman, Spectral clustering based on local linear approximations, *Electron. J. Stat.*, **5** (2011), 1537–1587.
3. P. Daugulis, A note on a generalization of eigenvector centrality for bipartite graphs and applications, *Networks*, **59** (2012), 261–264.
4. D. J. Griffiths, *Introduction to Quantum Mechanics* (2nd edition), Prentice Hall, (2004).
5. F. Laloe, *Do We Really Understand Quantum Mechanics* (2nd edition), Cambridge University Press, (2019).
6. M. V. Diudea, I. Gutman, J. Lorentz, *Molecular Topology*, Nova Science Publishers, (2001).
7. G. Bieri, J. D. Dill, E. Heilbronner, A. Schmelzer, Application of the equivalent bond orbital model to the C2s-Ionization energies of saturated hydrocarbons, *Helv. Chim. Acta.*, **60** (1977), 2234–2247.
8. E. Heilbronner, A simple equivalent bond orbital model for the rationalization of the C2s-Photoelectron spectra of the higher n-Alkanes, in particular of polyethylene, *Helv. Chim. Acta.*, **60** (1977), 2248–2257.

9. H. Gunthard, H. Primas, Zusammenhang von Graphentheorie und MO-Theorie von Molekeln mit systemen konjugierter bindungen, *Helv. Chim. Acta.*, **39** (1956), 1645–1653.
10. S. Meenakshi, S. Lavanya, A survey on energy of graphs, *Ann. Pure Appl. Math.*, **8** (2014), 183–191.
11. G. Indulal, A. Vijaykumar, Energies of some non-regular graphs, *J. Math. chem.*, **42** (2007), 377–386.
12. M. Jooyandeh, D. Kiani, M. Mirzakhani, Incidence energy of a graph, *MATCH. Commun. Math. Comput. Chem.*, **62** (2009), 561–572.
13. I. Gutman, The energy of a graph, *Ber. Math. Stat. Sect. Forschungszent. Graz*, **103** (1978), 1–22.
14. I. Gutman, B. Zhou, Laplacian energy of a graph, *Lin. Algebra Appl.*, **414** (2006), 29–37.
15. B. Zhou, I. Gutman, On Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.*, **57** (2007), 211–220.
16. I. Gutman, G. Indulal, A. Vijaykumar, On distance energy of graphs, *MATCH Commun. Math. Comput. Chem.*, **60** (2008), 461–472.
17. I. Gutman, X. Li, Y. Shi, *Graph Energy*, Springer, (2012).
18. V. Nikiforov, The energy of graphs and matrices, *Jour. Math. Anal. Appl.*, **326** (2007), 1472–1475.
19. D. Cvethovic, P. Rowlinson, K. Simic, Signless Laplacians of finite graphs, *MATCH Commun. Math. Comput. Chem.*, **57** (2007), 211–220.
20. T. Turaci, The average lower 2-domination number of wheels related graphs and an algorithm, *Math. Comput. Appl.*, **21** (2016), 1–9.
21. A. Aytac and T. Turaci, Vertex vulnerability parameter of Gear Graphs, *Int. J. Found. Comput. Sci.*, **22** (2011), 1187–1195.
22. J. B. Liu, M. Munir, A. Yousaf, A. Naseem, K. Ayub, Distance and Adjacency energies of Multi-Level wheel networks, *Mathematics*, **7** (2019), 1–9.
23. J. B. Liu, X. F. Pan, F. T. Hu, Asymptotic Laplacian-energy-like invariant of lattices, *Appl. Math. Comput.*, **253** (2015), 205–214.
24. J. B. Liu, X. F. Pan, Asymptotic incidence energy of lattices, *Phy. A*, **422** (2015), 193–202.
25. I. Tomescu, I. Javaid, Slamini, On the partition dimension and connected partition dimension of wheels, *Ars Comb.*, **84** (2007), 311–317.
26. H. M. A. Siddique, H. Imran, Computing the metric dimension of wheel related graphs, *Appl. Math. Comput.*, **242** (2014), 624–632.
27. Z. Hussain, S. M. Kang, M. Rafique, M. Munir, U. ALi, A. Zahid, et al., Bounds for partition dimension of m -Wheels, *Open Phy.*, **17** (2019), 340–344.



AIMS Press

©2020 the Author(s), licensee AIMS Press. This is an open access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>)