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Spectra and energy of the vertex labeled complement of graphs

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Abstract

For any graph, the sum of the absolute values of the eigenvalues of the adjacency matrix is known as the energy of graph. In this paper, we find the spectrum and energy of vertex labeled complement of distinct graphs along with their bounds and extend it to three applications for the complements of some alkanes.

Keywords: Vertex labeled graph, complement of a graph, spectrum, energy, alkanes

2020 MSC: 05C50

1. Introduction

For fundamental notions and terminology we refer [8]. Throughout the work we consider undirected simple graph (for an example, see Figure 1).

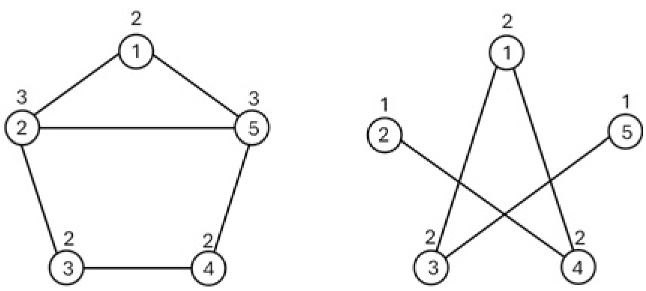

Figure 1. An undirected simple graph and its complement

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Let $\Gamma(V, E)$ be a graph. The complement $\overline{\Gamma}(V, E')$ of $\Gamma(V, E)$, has the same vertex set as Γ, but two vertices are adjacent in $\overline{\Gamma}(V, E')$ if and only if they are not adjacent in Γ. The union of the respective edge sets, that is $E(\Gamma) \cup E'(\overline{\Gamma}) = E(K_n(\Gamma))$ which is the edge set of complete graph with vertex set $V(\Gamma)$, that is, of K_n. There are many results on the complements of graphs, mostly relating them to the given graph. In particular, there is a class of results giving the relations for different graph parameters of the graph Γ and its complement $\overline{\Gamma}$ called as Nordhaus-Gaddum type results (*cf.* [10]).

Rosa [14] initiated the labeling of graphs which is actually a function f that connects the set of vertices V and the set of positive integers. For any two vertices $u, v \in V$, one may assign each edge $uv \in E$ with a label depending on the labels $f(u)$ and $f(v)$. We may refer, for instance, [16, 17] for some recent results.

Gutman [7] introduced the concept of energy of graph as the sum of the absolute values of the eigenvalues of the adjacency matrix of the given graph. Various energies of graphs like Harary energy of a graph [6], Laplacian energy [5], Energy of binary labeled Graphs [1], Vertex labeled graph energy [12], Resistance-distance energy of a graph [3] Partition Laplacian energy of a graph [11], Laplacian-energy-like invariant [4] etc exist in literature.

In this paper, we extended the work [12] of vertex labeled graph energy to vertex labeled complement of graphs.

2. Vertex labeled complement of graphs and their energy

The matrix corresponding to vertex labeled complement of a graph is defined as

$$M\left[V_L(\overline{\Gamma})\right] = \begin{cases} L(v_i) + L(v_j), & \text{if there is a path between } v_i \text{ and } v_j \\ 0, & \text{if there is no path between } v_i \text{ and } v_j \text{ or if } v_i = v_j \end{cases}$$

with vertices v_i , v_j labeled using their degrees and denoted by $L(v_i)$, $L(v_j)$, respectively.

Let $\eta_1, \eta_2, \cdots, \eta_r$ be the eigenvalues of the matrix of vertex labeled complement of graph $V_L(\overline{\Gamma})$ then the energy of vertex labeled complement of graph is defined as $\mathcal{E}\left[V_L(\overline{\Gamma})\right] = \sum_{i=1}^{r} |\eta_i|$.

The vertex labeled complement of graph spectrum consists of distinct eigenvalues $\eta_1 > \eta_2 > \cdots > \eta_r$ with multiplicities $m_1, m_2, \ldots, m_r$, respectively, and defined by

$$\operatorname{Spec}\left[V_L(\overline{\Gamma})\right] = \begin{pmatrix} \eta_1 & \eta_2 & \cdots & \eta_r \\ m_1 & m_2 & \cdots & m_r \end{pmatrix}.$$

2.1. *Results of the vertex labeled complement of graphs*

Theorem 2.1. *If the eigenvalues of $V_L(\overline{\Gamma})$ are $\eta_1 > \eta_2 > \cdots > \eta_r$, then*

(i) $\sum_{i=1}^{r} \eta_i = 0.$

(ii) $\sum_{i=1}^{r} \eta_i^2 = 2 \sum_{i<j} \left[L(v_i) + L(v_j)\right]^2 = 2B,$

where $B = \sum_{i<j} \left[L(v_i) + L(v_j)\right]^2.$

Proof. (i) In the matrix of vertex labeled complement graph $V_L(\overline{\Gamma})$, diagonal entries are zero, therefore their sum is zero. Hence $\sum_{i=1}^{p} \eta_i = 0$.

(ii) The sum of squares of eigenvalues of $V_L(\overline{\Gamma})$ is twice the sum of eigenvalues of $[V_L(\overline{\Gamma})]^2$:

$$\begin{aligned}\sum_{i=1}^{p}\eta_i^2 &= \sum_{i=1}^{p}\sum_{j=1}^{p}u_{ij}\,u_{ji}\\ &= 0+2\sum_{i<j}(u_{ij})^2\\ &= 2\sum_{i<j}\Big[L(v_i)+L(v_j)\Big]^2\\ &= 2B.\end{aligned}$$

□

Theorem 2.2. *Let the initial three coefficients of characteristic polynomial of $V_L(\overline{\Gamma})$ be c_0, c_1 and c_2. Then* **(i)** $c_0 = 1$, **(ii)** $c_1 = 0$, **(iii)** $c_2 = -B$.

Proof. (i) By definition, $\overline{\Gamma}(\eta, x) = \det[\eta I - B]$. Therefore $c_0 = 1$.

(ii) $c_1 = (-1)^1 \cdot \text{trace}(\overline{\Gamma}) = -1 \cdot 0 = 0$.

(iii) By definition,

$$\begin{aligned}c_2 &= \sum_{1\le i<j\le p}\begin{vmatrix} a_{ii} & a_{ij}\\ a_{ji} & a_{jj}\end{vmatrix}\\ &= \sum_{1\le i<j\le p}(a_{ii}a_{jj}-a_{ij}a_{ji})\\ &= \sum_{1\le i<j\le p}a_{ii}a_{jj}-\sum_{1\le i<j\le p}a_{ij}^2 = 0-B=-B.\end{aligned}$$

□

As per McClelland's inequalities, we have the following bounds for $\mathcal{E}[V_L(\overline{\Gamma})]$, (*cf.* [9]).

Theorem 2.3. *If $\overline{\Gamma}$ is the complement of a graph Γ with p vertices, then the upper bound for energy of $V_L(\overline{\Gamma})$ is*

$$\mathcal{E}\Big[V_L(\overline{\Gamma})\Big] \le \sqrt{2pB}.$$

Proof. Let $\eta_1 > \eta_2 > \cdots > \eta_n$ be the eigenvalue of $V_L(\overline{\Gamma})$, then by using Cauchy-Schwarz inequality, we have

$$\left[\sum_{i=1}^{p}u_iv_i\right]^2 \le \left[\sum_{i=1}^{p}u_i^2\right]\left[\sum_{i=1}^{p}v_i^2\right].$$

Choose $u_i = 1, v_i = |\eta_i|$. By Theorem 2.1

$$\left[\sum_{i=1}^{p}|\eta_i|\right]^2 \le \left[\sum_{i=1}^{p}1\right]\left[\sum_{i=1}^{p}|\eta_i|^2\right] = p\sum_{i=1}^{p}\eta_i^2$$

$$[\mathcal{E}\Big(V_L(\overline{\Gamma})\Big]^2 \le p2B.$$

Hence the result follows. □

Theorem 2.4. *If $\overline{\Gamma}$ is the complement of a graph Γ with p vertices, then the lower bound for energy of $V_L(\overline{\Gamma})$ is*

$$\mathcal{E}\Big[V_L(\overline{\Gamma})\Big] \ge \sqrt{2B + p(p-1)\tau^{\frac{2}{p}}},$$

where $\tau = \Big|\det V_L(\overline{\Gamma})\Big|$ of $\overline{\Gamma}$.

Proof. By definition, we have

$$\begin{aligned}\left[\mathcal{E}\left(V_L(\overline{\Gamma})\right)\right]^2 &= \left[\sum_{i=1}^{p}|\eta_i|\right]^2 = \left[\sum_{i=1}^{p}|\eta_i|\right]\left[\sum_{j=1}^{p}|\eta_j|\right]\\ &= \sum_{i=1}^{p}|\eta_i|^2 + \sum_{i\neq j}|\eta_i||\eta_j|.\end{aligned}$$

From the inequality of arithmetic and geometric means

$$\frac{1}{p(p-1)}\sum_{i\neq j}|\eta_i||\eta_j| \geq \left[\prod_{i\neq j}|\eta_i||\eta_j|\right]^{\frac{1}{p(p-1)}}.$$

Therefore,

$$\begin{aligned}\left[\mathcal{E}\left(V_L(\overline{\Gamma})\right)\right]^2 &\geq \sum_{i=1}^{p}|\eta_i|^2 + p(p-1)\left[\prod_{i\neq j}|\eta_i||\eta_j|\right]^{\frac{1}{p(p-1)}}\\ &\geq \sum_{i=1}^{p}|\eta_i|^2 + p(p-1)\left[\prod_{i=1}^{p}|\eta_i|^{2(p-1)}\right]^{\frac{1}{p(p-1)}}\\ &= \sum_{i=1}^{p}|\eta_i|^2 + p(p-1)\left|\prod_{i=1}^{p}\eta_i\right|^{\frac{2}{p}}\\ &= 2B + p(p-1)\tau^{\frac{2}{p}}.\end{aligned}$$

Hence the result follows. □

We now extended this concept to find energy of different vertex labeled complement of graphs.

2.2. *Energy of the vertex labeled complement of graphs*

First we need an example:

Example 2.5. Let $V_L(\overline{\Gamma})$ be the vertex labeled complement of graph Γ with 5 vertices. Then its energy is given by

$$\mathcal{E}\left[V_L(\overline{\Gamma})\right] = 10 + 6\sqrt{7}.$$

To see this, let the vertex set of the graph Γ and its complement graph $\overline{\Gamma}$ be $V = \{1, 2, 3, 4, 5\}$ with $p = 5$ and in both the graphs the vertices are labeled with number of edges incident to them respectively (see Figure 1). Thus the adjacency matrix of the vertex labeled graph $\overline{\Gamma}$ is given by

$$V_L(\overline{\Gamma}) = \begin{bmatrix}0 & 3 & 4 & 4 & 3\\ 3 & 0 & 3 & 3 & 2\\ 4 & 3 & 0 & 4 & 3\\ 4 & 3 & 4 & 0 & 3\\ 3 & 2 & 3 & 3 & 0\end{bmatrix}.$$

Its characteristic polynomial is

$$[\eta^2 - 10\eta - 38][\eta + 2][\eta + 4]^2 = 0$$

with spectrum

$$\text{Spec}\left[V_L(\overline{\Gamma})\right] = \begin{pmatrix} 5 - 3\sqrt{7} & 5 + 3\sqrt{7} & -2 & -4\\ 1 & 1 & 1 & 2\end{pmatrix}.$$

Thus, the energy of vertex labeled complement of graph Γ is

$$\begin{aligned}\mathcal{E}\left[V_L(\overline{\Gamma})\right] &= \left|5-3\sqrt{7}\right|(1)+\left|5+3\sqrt{7}\right|(1)+\left|-2\right|(1)+\left|-4\right|(2)\\ &= 10+6\sqrt{7}.\end{aligned}$$

Theorem 2.6. *Let $\overline{C_p}$ be the complement of a cycle graph with $p \geq 5$. Then the energy of vertex labeled complement of C_p graph is given by*

$$\mathcal{E}\left[V_L(\overline{C_p})\right] = 4p^2 - 16p + 12.$$

Proof. Let $V = \{v_1, v_2, \cdots, v_p\}$ be the vertex set of a vertex labeled complement graph $\overline{C_p}$ of a cycle graph with $p \geq 5$. Then

$$V_L(\overline{C_p}) = \begin{bmatrix} 0 & 2p-6 & 2p-6 & \dots & 2p-6 & 2p-6\\ 2p-6 & 0 & 2p-6 & \dots & 2p-6 & 2p-6\\ 2p-6 & 2p-6 & 0 & \dots & 2p-6 & 2p-6\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 2p-6 & 2p-6 & 2p-6 & \dots & 0 & 2p-6\\ 2p-6 & 2p-6 & 2p-6 & \dots & 2p-6 & 0 \end{bmatrix}.$$

Its characteristic polynomial is

$$[\eta-(2p^2-8p+6)][\eta+2p-6]^{p-1}=0$$

with spectrum

$$\text{Spec}\left[V_L(\overline{C_p})\right] = \begin{pmatrix} 2p^2-8p+6 & -2p+6\\ 1 & p-1 \end{pmatrix}.$$

Thus, the energy of vertex labeled complement of a cycle graph is

$$\begin{aligned}\mathcal{E}[V_L(\overline{C_p})] &= \left|2p^2-8p+6\right|(1)+\left|-2p+6\right|(p-1)\\ &= 4p^2-16p+12.\end{aligned}$$

□

Theorem 2.7. *Let $\overline{S_p^0}$, be complement of a crown graph with $p \geq 2$ having $2p$ vertices. Then the energy of vertex labeled complement of S_p^0 graph is given by*

$$\mathcal{E}[V_L(\overline{S_p^0})] = 8p^2 - 4p.$$

Proof. Let $V = \{u_1, u_2, \cdots, u_p, v_1, v_2, \cdots, v_p\}$ be vertex set of vertex labeled complement graph $\overline{S_p^0}$ of a crown graph of order $2p$. Then

$$V_L(\overline{S_p^0}) = \begin{bmatrix} 0 & 2p & 2p & \dots & 2p & 2p\\ 2p & 0 & 2p & \dots & 2p & 2p\\ 2p & 2p & 0 & \dots & 2p & 2p\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 2p & 2p & 2p & \dots & 0 & 2p\\ 2p & 2p & 2p & \dots & 2p & 0 \end{bmatrix}.$$

Its characteristic polynomial is

$$[\eta-(4p^2-2p)][\eta+2p]^{2p-1}=0$$

with spectrum

$$\text{Spec}\left[V_L(\overline{S_p^0})\right] = \begin{pmatrix} 4p^2-2p & -2p\\ 1 & 2p-1 \end{pmatrix}.$$

Thus, the energy of the vertex labeled complement of a crown graph is

$$\begin{aligned}\mathcal{E}[V_L(\overline{S_p^0})] &= \left| 4p^2 - 2p \right| (1) + \left| -2p \right| (2p-1) \\ &= 8p^2 - 4p.\end{aligned}$$

□

Theorem 2.8. *Let $\overline{C_nH_{2n+2}}$, $n = \{2,3,4\}$, be the complement graph of alkane graph with $p = 3n+2$ vertices. Then the energy of vertex labeled complement of C_nH_{2n+2} graph is given by*

$$\mathcal{E}[V_L(\overline{C_nH_{2n+2}})] = \sqrt{p^4 - 10p^3 + 145p^2 - 1440p + 4965} + 2p^2 - 10p + 18.$$

Proof. Let $V = \{a_1, a_2, \cdots, a_r, b_1, b_2, \cdots, b_s\}$ be the vertex set of vertex labeled complement graph $\overline{C_nH_{2n+2}}$ of an alkane graph of order $p = 3n+2$, $n = \{2,3,4\}$ with $r + s = p$, a_i representing carbon atoms and b_i representing hydrogen atoms.

Case (i): Let $n = 2$ in $\overline{C_nH_{2n+2}}$. The vertex labeled complement graph $\overline{C_2H_6}$ of Ethane has order 8 and size 21. Its characteristic polynomial is

$$[\eta^2 - 66\eta - 612][\lambda + 12]^5[\eta + 6] = 0$$

with spectrum

$$\text{Spec}\left[V_L(\overline{C_2H_6})\right] = \begin{pmatrix} 33 - 9\sqrt{21} & 33 + 9\sqrt{21} & -6 & -12 \\ 1 & 1 & 1 & 5 \end{pmatrix}.$$

Thus, the energy of the vertex labeled complement graph of Ethane is

$$\mathcal{E}\left[V_L(\overline{C_2H_6})\right] = 148.486.$$

Case (ii): $n = 3$ in $\overline{C_nH_{2n+2}}$. The vertex labeled complement graph $\overline{C_3H_8}$ of Propane has order 11 and size 45. Its characteristic polynomial is

$$[\eta^2 - 150\eta - 2376][\eta + 12]^2[\eta + 18]^7 = 0$$

with spectrum

$$\text{Spec}\left[V_L(\overline{C_3H_8})\right] = \begin{pmatrix} 75 - 3\sqrt{889} & 75 + 3\sqrt{889} & -12 & -18 \\ 1 & 1 & 2 & 7 \end{pmatrix}.$$

Thus, the energy of the vertex labeled complement graph of Propane is

$$\mathcal{E}\left[V_L(\overline{C_3H_8})\right] = 328.914.$$

Case (iii): $n = 4$ in $\overline{C_nH_{2n+2}}$. The vertex labeled complement graph $\overline{C_4H_{10}}$ of Butane has order 14 and size 78. Its characteristic polynomial is

$$[\eta^2 - 270\eta - 5976][\eta + 18]^3[\eta + 24]^9 = 0$$

with spectrum

$$\text{Spec}\left[V_L(\overline{C_4H_{10}})\right] = \begin{pmatrix} 135 - 3\sqrt{(2689)} & 135 + 3\sqrt{(2689)} & -18 & -24 \\ 1 & 1 & 3 & 9 \end{pmatrix}.$$

Thus, the energy of the vertex labeled complement graph of Butane is

$$\mathcal{E}\left[V_L(\overline{C_4H_{10}})\right] = 581.1334.$$

□

3. Conclusion

In the light of several applications of graphs to various fields, we have extended our work to evaluate the spectra and energy of some alkanes along with properties and bounds. Alkanes and similar chemical structures are very important raw materials for chemical industry and a main component of gasoline and lubricating oils (*cf.* [2]). In future we try to extended our work in line with applications to benefit field of graph theory as well as the chemical industry.

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