Nullity and Energy Bounds of Central Graph of Smith Graphs

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Abstract: A smith graph G is a graph whose at least one eigenvalue is 2. The nullity (G) of a graph G is the multiplicity of the eigenvalue 0 in the spectrum of adjacency matrix of graph A (G). Energy of the graph is the sum of the absolute values of the Eigen values of the adjacency matrix G. Central graph C (G) of graph G is obtained by subdividing each edge exactly once and joining all the non adjacent vertices of graph G. We have evaluated the nullity and the energy bounds of the central graph of smith graphs. By Huckel molecular Orbital theory, these spectral properties are applicable for determining the stability of unsaturated conjugate hydrocarbons which are isomorphic to central graph of smith graphs.

Keywords: Smith graph, Central graph, Nullity, Energy, Huckel molecular Orbital theory

1. Introduction

Spectral graph theory is the study of properties of graphs in relationship to the characteristic polynomials, Eigen values and eigenvectors of matrices associated with graphs. In a theory of graph spectra, some special types of graphs are studied in detail and their characteristics are well known and summarized in [CvDSa]. Here we discussed the smith graphs. Smith graphs are Cₙ (n ≥ 3), Wₙ (n ≥ 6), S₅ = K₁,₄, H₇, H₈ and H₉.

The central graph C (G) of a graph G is obtained by subdividing each edge of G exactly once and joining all the nonadjacent vertices of G.

Here, we have evaluated the nullity of a special type of graphs and also elaborated energy bounds. Let G be a graph of order n, having vertex set V (G) and edge set E (G). Let A (G) be the adjacency matrix of G, where

$$A(G) = \begin{cases} 1, & \text{if } v_i \text{ is adjacent to } v_j \\ 0, & \text{if } v_i \text{ is not adjacent to } v_j \end{cases}$$

$$A[G] = \begin{bmatrix} 0 & 1 & 1 & 0 & \cdots & 1 \\ 1 & 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ 1 & 1 & 1 & 1 & \cdots & 1 \end{bmatrix}_{(n \times n)}$$
A scalar $\lambda$ is called an eigenvalue of the square matrix $A(G)$ if there exist a nonzero vector $X$ such that $AX = \lambda X$, where $X$ is called an eigenvector corresponding to the eigenvalue $\lambda$. In other words, Eigen values are the set of scalars which is associated with a characteristic equation of adjacency matrix of graph $G$ that is $|A- \lambda I| = 0$, where $I$ is the identity matrix.

Nullity of G is the zero multiplicity of an eigenvalue in the spectrum of $A(G)$. It is firstly introduced by Gutman in his paper.

The chemical importance of this graph spectrum based invariant lies in the fact, that within the Huckel molecular orbital model, if $\eta(G) > 0$ for the molecular graph $G$, then the corresponding chemical compound is highly reactive and unstable or nonexistent and if $\eta(G) = 0$ then the respective molecule is predicted to have a stable, closed-shell, electron configuration and low chemical reactivity.

In 1940's energy introduced by chemistry. Ivan Gutman, (1978) interpreted the energy of graph in first time. However, the inspirations for his definition vision much earlier, in the 1930's, when Erich Huckel recommended the famous Huckel Molecular Orbital Theory. Huckel's method permits chemists to approximate energies related with $\pi$-electron orbital's in a special group of molecules called conjugated hydrocarbons. The method assumes that the Hamiltonian operator is a simple linear combination of certain orbital, and given the time-independent Schrodinger equation to solve for the energies desired (2012).

Gunthard, H. H. and Primas, H. (1956) realized that the matrix is applicable in the Huckel method is a first degree polynomial of the adjacency matrix of a certain graph related to the molecule being studied.

Moreover, under certainly reasonable speculation about the molecule, its total $\pi$-electron energy can be written as the energy of the graph is the sum of the absolute values of the Eigen values $\lambda$ of the adjacency matrix $A(G)$ that is $E(G) = \sum_{i=1}^{n} |\lambda_i|$ is related to the total $\pi$-electron energy in a molecular graph.

We have appraised the energy bounds of the graph with the help of Schwartz inequality. Let $a_1, \ldots, a_n$ and $b_1, \ldots, b_n$ be the two sequences. Then

$$\left( \sum_{i=1}^{n} a_i b_i \right)^2 \leq \left( \sum_{i=1}^{n} |a_i|^2 \right) \left( \sum_{i=1}^{n} |b_i|^2 \right)$$

Rest of the paper in section 2 we have given related work to nullity and energy of graphs. We use one proposition in this paper. we have mentioned in section 3. In section 4, we have determined new results on the nullity of the central graph of smith graphs. In section 5, we have evaluated energy bounds of central graph of smith graph. We have concluded the results in section 6.

2. Literature Review

Spectral graph theory vision during the two decades starting from 1940 to 1960. "The theory of graph spectra" written by Cvetkovic, D. M. et al. (1980), has included the monograph of the research area of spectral graph theory and further updated newer results in the theory of graph spectra (1989). In the preceding 9 -10 years, many developments in this arena such as Lubotzky, A. et al. (1988) gave isometric properties of expander graphs. Currently developed spectral techniques are more powerful and convenient for well-established graph. Gutman, I. (2001) has shown in his paper that nullity of the line graph of the tree that is $\eta(L(T))$ at most one. Boravicanin, B. and Gutman, I. (2011) in their paper related to the nullity of graphs, explained the chemical importance of graph- spectrum based on Huckel molecular orbital theory and recently obtained general mathematical results on the nullity of graphs $\eta(G)$. Barrette, W. et al. (2014) have found the maximum nullity of a complete subdivision graph. Gu, R. et al. (2014) have done the research on randic incidence energy of graphs. Sharaf, K. R. and Rasad, K. B. (2014) gave results on the nullity of expanded graphs and Sharaf, K. R. and Ali, D. A. (2014) have given nullity of t- tuple graphs. S. (2014) has shown the expression of the nullity set of unicyclic graphs depend on the extremal nullity.

Coulson, C. A. and et al. (1978) explained some graphical aspects of Huckel theory and also explained the energy level of the graph. Biggs, N. (1993) discussed the applications of linear algebra and matrix theory in Algebraic graph theory. Gutman, I. (2001) presented fundamental mathematical results on E and relation between E(G) and characteristic polynomial of G and bounds for E. Bo, Z.(2004) presented upper bound for the energy of a graph in terms of a degree sequence and specified maximal energy graph and maximal energy bipartite graph. Adiga, C. and et al. (2007) determined the several classes of graphs such as biregular, molecular graphs, trigraphs graphs satisfy the condition $E(G) > n$. Gutman, I. and et al. (2012) explicated the chemical origin of the graph energy concept and briefly survey of applications of total $\pi$-electron energy. Gutman, I. and et al. (2015) shown that for a fixed value of $n$, both the spectral radius and the energy of complete p- partite graphs are minimal for complete split graph $CS(n, p-1)$ and are maximal for Turan graph $T(n, p)$. Song Y. Z. and et al. (2015) proved that the nullity of the bipartite graph that is $\eta(G) = |G|-2- 2 \sum_{i=1}^{n} |X|$ of $A(G)$, if $G$ is a reduced bipartite graph.

3. Preposition

Proposition 3.1: Let G be a graph and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the Eigen values of adjacency matrix $A(G)$, then

$$\sum_{i=1}^{n} \lambda_i^2 = 2 \cdot \text{number of edges}$$

4. Nullity of Central graph of Smith graphs

We will discuss the nullity of central Graph of different types of smith graph out of these many are nonsingular.
**Theorem 4.1:** Nullity of central graph of smith graph $W_n; n \geq 6$ is zero, that is $\eta [C(W_n)] = 0 \ \forall \ n \geq 6$.

**Proof:** Consider a smith graph $W_n$ with vertex set $V = \{v_1, v_2, v_3, \ldots, v_n\}$ and edge set $E = \{e_1, e_2, e_3, \ldots, e_{n-1}\}$ respectively. Then, $C(W_n)$ has vertex set $\{v_1, u_1, v_2, u_2, \ldots, v_{n-2}, u_{n-1}, v_{n-1}, u_{n-1}, v_n\}$ and edge set $\{e_1, e'_1, e_2, e'_2, \ldots, e_{n-1}, e'_{n-1}, \ldots, e_{12}, e_{14}, \ldots, e_{17}, e_{24}, e_{25}, \ldots, e_{27}, \ldots, e_{3n}, e_{37}\}$.

**Figure 3:** $C(W_n)$

Now the total number of vertices $p$ in $C(W_n)$ = number of vertices in $(W_n)$ + number of edges in $(W_n)$ = $n + (n-1) = 2n-1$. The total number of edges $q$ in $C(W_n)$ = $2 \times$ (number of edges in $W_n$) + number of edges between non-adjacent vertices in $W_n$ = $2(n-1) +$ number of edges in $K_n$ - number of edges in $W_n$ = $2(n-1) + \frac{n(n-1)}{2} - (n-1) = \frac{(n-1)(n+2)}{2}$. Now we find the nullity of graph $C(W_n)$.

Firstly we construct adjacency matrix

$$[a_{ij}]_{(2n-1)(2n-1)} = \begin{cases} 1, & \text{if } v_i \text{ is adjacent to } v_j \\ 0, & \text{if } v_i \text{ is not adjacent to } v_j \end{cases}$$

$$A[C(W_n)] = \begin{bmatrix} 0 & 1 & 1 & 0 & \ldots & \ldots & 1 \\ 1 & 0 & 0 & 0 & \ldots & \ldots & 1 \\ 1 & 0 & 0 & 1 & \ldots & \ldots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & 1 & 0 \\ 1 & 1 & 1 & 1 & \ldots & 1 & 0 \end{bmatrix}_{(2n-1)(2n-1)}$$

Now we apply elementary row operation for finding the nullity of the graph. Nullity of graph = $|G| - r(A(G))$, where $r(A(G))$ is the rank of matrix. Then, $r(A(G)) = \text{number of non-zero rows in the row reduced form of matrix} = (2n-1)$. Then the nullity of graph = $|C(W_n)| - r(A(G)) = (2n-1) - (2n-1) = 0$.

Therefore, $\eta [C(W_n)] = 0 \ \forall \ n \geq 6$.

**Theorem 4.2:** Nullity of central graph of smith graph $H_7$ is zero, that is $\eta [C(H_7)] = 0$.

**Proof:** Consider a smith graph $H_7$ with vertex set $V = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$ and edge set $E = \{e_1, e_2, e_3, e_4, e_5, e_6\}$ respectively. Then, $C(H_7)$ has vertex set $\{v_1, u_1, v_2, u_2, \ldots, v_6, u_6, v_6, u_6, v_7\}$ and edge set $\{e_1, e_1, e_2, e_2, \ldots, e_6, e_6, e_{19}, e_{13}, e_{14}, \ldots, e_{26}, e_{25}, \ldots, e_{27}, \ldots, e_{3n}, e_{37}\}$.

**Figure 4:** $C(H_7)$

Number of vertices in $H_7$ + number of edges in $H_7$ = 13 and the total number of edges in $C(H_7)$ = $2 \times$ (number of edges in $H_7$) + number of edges between non-adjacent vertices in $H_7$ = $12 +$ number of edges in $K_7$ - number of edges in $H_7$ = $12 + \frac{7(7-1)}{2} - 6 = 27$. Now we find the nullity of graph $C(H_7)$. Then, we construct the adjacency matrix $A = [a_{ij}]_{13 \times 13}$.

The $A[C(H_7)]$ of the $13 \times 13$ order

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}_{13 \times 13}$$

We apply elementary row operation for determined the nullity of graph. Nullity of graph = $|G| - r(A(G))$, where $r(A(G))$ is the rank of matrix. The rank of graph = number of non-zero row in the row reduced form of matrix = 13. Therefore, $\eta [C(H_7)] = 0$.

**Theorem 4.3:** Nullity of central graph of smith graph $H_8$ is zero. i.e. $\eta [C(H_8)] = 0$.
Proof: Consider a smith graph $H_8$ with vertex set $V = \{v_1, v_2, \ldots, v_8\}$ and edge set $E = \{e_1, e_2, \ldots, e_7\}$ respectively. Then, $C(H_8)$ has vertex set $\{v_1, u_1, v_2, u_2, \ldots, u_7, v_8\}$ and edge set $\{e_1, e_2, e_2, e_3, e_4, e_5, e_6, e_7, e_8, e_{25}, \ldots, e_{28}\}$.

Now the total number of vertices in $C(H_8)$ is the number of vertices in $H_8$ + the number of edges in $H_8 = 15$ and the total number of edges in $C(H_8)$ is $(2 \times \text{number of edges in } H_8) + \text{number of edges between non-adjacent vertices in } H_8 = 14 + \text{number of edges in } K_8 - \text{number of edges in } H_8 = 14 + \frac{8(8-1)}{2} = 35$. Now we find the nullity of graph $C(H_8)$.

Firstly we construct the adjacency matrix $A = \{a_{ij}\}_{15 \times 15}$. We apply elementary row operation for rank. Nullity of graph $\eta = |(G)| - r(A(G))$, where $r(A(G))$ is the rank of matrix. Then, the rank of matrix = number of non-zero row in the row reduced form of matrix = 15. Therefore, $\eta = 0$.

Theorem 4.4: Nullity of central graph of smith graph $S_5$ is zero. i.e. $\eta [C(S_5)] = 0$.

Proof: Consider a smith graph $S_5$ with vertex set $V_1 = \{v_1\}$ and $V_2 = \{u_1, u_2, u_3, u_4\}$ and edge set $E = \{e_1, e_2, e_3, e_4\}$ respectively. Then, $C(S_5)$ vertex set $\{v_1, w_1, u_1, w_2, u_2, w_3, u_3, w_4, u_4\}$ and edge set $\{e_1, e_1, e_2, e_2, e_3, e_3, e_4, e_4, e_{12}, e_{13}, e_{14}, e_{23}, e_{24} \}$.

Now the total number of vertices in $C(S_5)$ = number of vertices in $S_5$ + number of edges in $S_5 = 9$ and the total number of edges in $C(S_5)$ = $2(\text{number of edges in } S_5) + \text{number of edges between non-adjacent vertices in } S_5 = 8 + \text{number of edges in } K_5 - \text{number of edges in } S_5 = 8 + \frac{5(5-1)}{2} = 14$. Now we find the nullity of graph $C(S_5)$.

Firstly we construct the adjacency matrix $A = \{a_{ij}\}_{9 \times 9}$. We apply elementary row operation for rank. Nullity of graph $\eta = |(G)| - r(A(G))$, where $r(A(G))$ is the rank of matrix. Then, the rank of matrix = number of non-zero row in the row reduced form of matrix = 15. Therefore, $\eta = 0$.

Theorem 4.5: Nullity of central graph of smith graphs $H_9$ is one. i.e. $\eta [C(H_9)] = 1$.

Proof: Consider a smith graph $H_9$ with vertex set $V = \{v_1, v_2, \ldots, v_9\}$ and edge set $E = \{e_1, e_2, \ldots, e_8\}$ respectively. Then, $C(H_9)$ has vertex set $\{v_1, u_1, v_2, u_2, \ldots, u_7, v_8\}$ and edge set $\{e_1, e_2, e_2, e_3, e_4, e_5, e_6, e_7, e_{13}, e_{14}, e_{15}, e_{16}, e_{24}, e_{25}, \ldots, e_{28}\}$.

Now the total number of vertices in $C(H_9)$ = number of vertices in $H_9$ + number of edges in $H_9 = 17$ and the total number of edges in $C(H_9)$ = $2(\text{number of edges in } H_9) + \text{number of edges between non-adjacent vertices in } H_9 = 16 + \text{number of edges in } K_9 - \text{number of edges in } H_9 = 16 + \frac{9(9-1)}{2} = 44$. Now we find the nullity of graph $C(H_9)$.

Firstly we construct the adjacency matrix $A = \{a_{ij}\}_{17 \times 17}$. We apply elementary row operation for rank. Nullity of graph $\eta = |(G)| - r(A(G))$, where $r(A(G))$ is the rank of matrix. Then, the rank of matrix = number of non-zero row in the row reduced form of matrix = 16. Therefore, $\eta = 1$.

Theorem 4.6: Nullity of central graph of smith graphs $C_n$ ; $n \geq 3$ are as follows:

\[
\eta[C(C_n)] = \begin{cases} 
0, & \text{if } n \text{ is an odd positive integer} \\
1, & \text{if } n \text{ is an even positive integer} 
\end{cases}
\]
Proof: Consider a smith graph $C_n$ with vertex set $V = \{v_1, v_2, v_3, \ldots, v_n\}$ and edge set $E = \{e_1, e_2, e_3, \ldots, e_n\}$ respectively. Then, $C(C_n)$ vertex set $\{v_1, u_1, v_2, u_2, \ldots, v_{n-2}, u_{n-1}, v_{n-1}, u_{n-1}, v_n\}$ and edge set $\{e_1, e'_1, e_2, e'_2, \ldots, e_n, e'_n, \ldots, e_{14}, e'_1(1)(n-1), e_{24}, e_{25}, \ldots, e_{2(n-1)}, \ldots, e_{(n-2)n}\}$.

Now the total number of vertices in $C(C_n)$ = number of vertices in $C_n$ + number of edges in $C_n = 2n$ and the total number of edges in $C(C_n) = 2(\text{number of edges in } C_n) + \text{number of edges between non-adjacent vertices in } C_n$ = $2n + \text{number of edges in } K_n - \text{number of edges in } C_n = 2n + \frac{n(n-1)}{2} - n = \frac{n(n+1)}{2}$. Now we find the nullity of graph $C(C_n)$. Firstly we construct the adjacency matrix $A = [a_{ij}]_{(n \times n)}$ of $C_n$, where $n$ is an odd positive integer. Then the nullity of $C(C_n) = |C(C_n)| - \text{Rank of matrix} = 0$ and if take $n$ is an even number of vertices then the nullity of $|C(C_n)| = |C(C_n)| - \text{Rank of matrix} = 1$.

5. Energy bounds of $C(W_n)$; $n \geq 6$, $C(H_n)$; $7 \leq n \leq 9$ and $C(S_5)$

Theorem 5.1: Let $C(W_n)$ $\forall n \geq 6$, $C(H_7)$, $C(H_8)$, $C(H_9)$, $C(S_5)$ be the central graph of smith graphs. We denote these graphs by $G$. Then the energy bound of $E(G)$ is

$E[\sqrt{(n-1)(n+2) + 2(2n-1)(n-1)|\det A(C(G))|^{2(2n-1)}}] \leq E[C(G)] \leq \sqrt{[(2n-1)(n-1)(n+2)]}$

Proof: Upper Bound: Energy of given graph $E^2[C(G)] = \sum_{\lambda_i} (\lambda_i)^2$

We use the Cauchy-Schwarz inequality to get

$E^2[C(G)] = (1, 1, \ldots, 1)\lambda_1, \lambda_2, \ldots, \lambda_{2n-1})$ to get

$E^2[C(G)] \leq (\lambda_1^2 + \lambda_2^2 + \ldots + \lambda_{2n-1}^2) (1 + 1 + \ldots + 1)$

Lower Bound: We use the arithmetic-geometric inequality

$E[C(G)] = \sum_{\lambda_i} |\lambda_i|$

$E^2[C(G)] = \left(\sum_{\lambda_i} |\lambda_i| \right)^2$

$E^2[C(G)] = \sum_{\lambda_i, \lambda_j} (\lambda_i^2 + \lambda_j^2) + \sum_{\lambda_i, \lambda_j} (\lambda_i \lambda_j)$

$E^2[C(G)] \geq (n-1)(n+2) + (2n-1)(2n-2)AM(\lambda_1, \lambda_2)$

Put the values of G. M. in equation (2) then we have

$E[\sqrt{(n-1)(n+2) + 2(2n-1)(n-1)|\det A(C(G))|^{2(2n-1)}}] \leq E[C(G)] \leq \sqrt{[(2n-1)(n-1)(n+2)]}$

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\[ E[C(G)] \leq (n-1)(n+2) + 2(2n-1)(n-1)|\det A(C(G))|^{\frac{1}{2n-1}} \]

Therefore,
\[ E[C(G)] \geq \sqrt{(n-1)(n+2) + 2(2n-1)(n-1)|\det A(C(G))|^{\frac{1}{2n-1}}} \]

Now, from equation (1) and (4) then we get
\[ \sqrt{(n-1)(n+2) + 2(2n-1)(n-1)|\det A(C(G))|^{\frac{1}{2n-1}}} \leq E[C(G)] \leq \sqrt{(2n-1)(n-1)(n+2)} \]

6. Conclusions

We have interpreted that any chemical compound is isomorphic to the central graph of smith graphs except central graph of smith graph \( H_9 \) and \( C_n \) where \( n \) is an even are stable, closed – shell electron configuration and have low chemical reactivity and if any chemical compound is isomorphic to \( C(H_9) \) and \( C(C_n) \) are unstable, open shell electron configuration and the respective compound is highly reactive.

References