Energy of Smith Graphs

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Abstract
In this manuscript, we have evaluated the energies of smith graphs. In the course of the investigation, we found that only one smith graph is hypo-energetic. Moreover we have also established the energy bounds for smith graph.

Keywords: Eigenvalue, energy, smith graphs, hypoenergetic graph.

1 Introduction
For all standard terminology and notations in graph theory and those in the theory of spectra of graphs, we refer the reader to Harary [3] and Cvetkovic et. al. [2], respectively. Particularly, all graphs considered in this paper are finite, simple, connected and undirected.

One of the current interests in mathematical chemistry, pharmacology, toxicology and biomedicinal chemistry is the prediction of pharmacological and biodynamic properties of molecules from their structure. The tacit assumption underlying this trend of research is that the structure of a molecule determines its behavior. To identify the certain classes of chemical compounds, one involves quite sophisticated mathematical techniques, where Graph Theory has

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come to play a major role. However, there are specific classes of graphs, which are isomorphic to unsaturated conjugate hydrocarbon compounds; for example, the smith graphs (i.e., a graph whose at least one eigenvalue is 2) \(W_m\) and \(C_m\) are isomorphic to unsaturated conjugate hydrocarbon compounds (for detail details see [1]). From the survey of the literature, we found the there are six kinds of smith graphs, viz., \(W_m\) \((m \geq 6)\), \(C_m\) \((m \geq 3)\), \(K_{1,4}\), \(H_7\), \(H_8\), and \(H_9\).

Let \(G = (V, E)\) be a simple graph with vertex set \(V = \{v_1, v_2, \ldots, v_m\}\) and edge set \(E = \{e_1, e_2, \ldots, e_n\}\). Let \(A(G)\) be the adjacency matrix of \(G\).

The energy \(E(G)\) of graph \(G\) is the sum of the absolute values of eigenvalues \(\lambda_1, \lambda_2, \ldots, \lambda_m\) of its adjacency matrix \(A(G)\). A graph \(G\) is said to be hypoenergetic if \(E(G) < m\), otherwise \(G\) is non-hypoenergetic. Let two non-isomorphic graphs \(G_1\) and \(G_2\) are said to be equienergetic graphs if \(E(G_1) = E(G_2)\) and if they have identical spectra then the graph is co-spectral equienergetic graphs, otherwise non co-spectral equienergetic graphs. Throughout the paper by \(S_m\), we mean a smith graph on \(m\) vertices and \(n\) edges. Except \(K_{1,4}\), other smith are the extended form of Dynkin graphs [5].

Motivated by the earlier study done in [4] on the energy of a graph, in this paper, we have focused on the energy of smith graphs. Moreover, we have characterized the smith graphs for which the energy bounds are attained in the Inequality \((m - 1) \leq E(S_m) \leq m + \left\lfloor \frac{n}{3} \right\rfloor\).

2 Main Results

In this section, we begin with the following existing results reported in [5], and will be found useful to derive new results. Later we will establish the results on energy bounds of smith graphs.

**Lemma 2.1** Let \(G\) be a graph and \(S(G)\) be the spectrum of \(G\). Then

(i) \(S(W_m) = \{2 \cos \frac{r\pi}{m-4} | r = 1, 2, \ldots, m - 5\} \cup \{-2, 0, 2\}\).

(ii) \(S(C_m) = \{2 \cos \frac{2r\pi}{m} | r = 0, 1, 2, \ldots, m - 1\}\).

(iii) \(S(H_7) = \{0, \pm 1, \pm 1, \pm 2\}\).

(iv) \(S(H_8) = \{2 \cos \frac{r\pi}{30} | r = 1, 7, 11, 13, 17, 19, 23, 29\}\).

(v) \(S(H_9) = \{2 \cos \frac{r\pi}{5} | r = 1, 2, 3, 4\} \cup \{0, \pm 1, \pm 2\}\).

(vi) \(S(K_{1,4}) = \{\pm 2, 0, 0, 0\}\).

In view of Lemma 2.1, the spectra of smith graph can be at most \(\{0, 0, 0, \ldots, 2, -2, \lambda_1, \lambda_2, \ldots, \lambda_i\}\). In general, the energy bounds on smith
graphs is given by the following result:

**Theorem 2.2** Let \( S_m \) be smith graph and \( E(S_m) \) be its energy. Then

\[
(m - 1) \leq E(S_m) \leq m + \left\lceil \frac{n}{3} \right\rceil.
\] (1)

**Proof.** Consider \( S_m \) be isomorphic to \( K_{1,4} \), whose spectrum is \(-2, 0, 0, 2\).
Clearly, \( E(K_{1,4}) \) is equal to 4, which is also equal to \((m - 1)\).
Now we consider \( S_m \) to be \( W_m \) \((m \geq 6)\). In view of Lemma 2.1, the spectrum of \( W_m \) is

\[
\{2 \cos \frac{r\pi}{m-4} | r = 1, 2, \ldots, m - 5\} U\{-2, 0, 0, 2\}.
\]

Thus, the energy of \( W_m \) is strictly greater than \((m - 1)\) and strictly less than to \( m + \left\lceil \frac{n}{3} \right\rceil\).
For the next case, if we consider \( S_m \) to be \( H_7 \), then

\[
(m - 1) < E(H_7) = (m + 1) < m + \left\lceil \frac{n}{3} \right\rceil
\]

\[
\Rightarrow (m - 1) < E(H_7) < m + \left\lceil \frac{n}{3} \right\rceil.
\]

Let \( S_m \) to be \( H_8 \). In view of Lemma 2.1, we get

\[
(m - 1) < E(H_8) < m + \left\lceil \frac{n}{3} \right\rceil.
\]

If we take \( S_m \) to be \( H_9 \), then again we get

\[
(m - 1) < E(H_9) < m + \left\lceil \frac{n}{3} \right\rceil.
\]

Finally, we take \( S_m \) to be \( C_m \) \((m \geq 3)\), for \( m = 6 \), \( E(C_m) \) attains the upper bound \( m + \left\lceil \frac{n}{3} \right\rceil \) and for other remaining values of \( m \) \((m \neq 6)\), the energy of \( C_m \) lies between \((m - 1)\) and \( m + \left\lceil \frac{n}{3} \right\rceil\).
From the above analysis, we conclude that

\[
(m - 1) \leq E(S_m) \leq m + \left\lceil \frac{n}{3} \right\rceil.
\]

\[\Box\]

At this stage we have the following problem:
Problem 2.3 Characterize the smith graphs for which the bounds are attained in the Inequality (1).

We answer to the above problem in the following theorems:

**Theorem 2.4** Let $S_m$ be smith graph and $E(S_m)$ be its energy. Then $E(S_m) = (m - 1)$ if and only if $S_m$ is isomorphic to $K_{1,4}$.

**Proof.** *Necessity:* Let us take $E(S_m) = (m - 1)$ and we have to show that the only smith graph will be $K_{1,4}$. We shall prove it by contradiction. Let us suppose that $S_m$ is not isomorphic to $K_{1,4}$. It means that it is isomorphic to either $W_m$ ($m \geq 7$) or $C_m$ ($m \geq 3$) or $H_7$ or $H_8$ or $H_9$. However none of the listed graphs have energy equal to $(m - 1)$. So, our assumption is wrong. Hence, $E(S_m) = (m - 1)$.

**Sufficiency:** Let $S_m$ be isomorphic to $K_{1,4}$. Clearly $K_{1,4}$ have 5 vertices and

$$E(K_{1,4}) = 4 = (m - 1).$$

Thus, the result follows. \qed

In other words we can say.

**Theorem 2.5** Let $S_m$ be smith graph and $E(S_m)$ be its energy. Then $E(S_m) = m + \lceil \frac{n}{3} \rceil$ if and only if $S_m$ is isomorphic to $C_6$.

**Proof.** For the necessity part, let us take $E(S_m) = m + \lceil \frac{n}{3} \rceil$ and we have to show that the only smith graph will be $C_6$. We shall prove it by contradiction. Let us suppose that $S_m$ is not isomorphic to $C_6$. It means that it is isomorphic to other smith graphs. However none of the graphs have energy equal to $m + \lceil \frac{n}{3} \rceil$. So, our assumption is wrong. Hence, $E(S_m) = m + \lceil \frac{n}{3} \rceil$.

For the sufficiency part, let $S_m$ be isomorphic to $C_6$. $C_6$ has the spectrum $\{-2, -1, -1, 1, 1, 2\}$, and hence $E(C_6) = 8$, which is equal to $m + \lceil \frac{n}{3} \rceil$. \qed

**Theorem 2.6** Let $S_m$ be smith graph and $E(S_m)$ be its energy. Then $E(S_m) = m$ if and only if $S_m$ is isomorphic to either $C_4$ or $W_6$.

**Proof.** *Necessity:* Let us take $E(S_m) = m$ and we shall show that the only smith graph is $C_4$ or $W_6$. Suppose to contrary that $S_m$ is neither isomorphic to $C_4$ nor $W_6$, it means $S_m$ can be isomorphic to other smith graphs. But, the energy of any of the smith graphs is not equal to $m$. So, our assumption is wrong. Hence, $S_m$ must be isomorphic to either $C_4$ or $W_6$.

**Sufficiency:** Let us assume that $S_m$ be isomorphic to $C_4$. Clearly, $C_4$ have 4
vertices and whose spectrum is \{-2, 0, 0, 2\}. Therefore, \(E(C_4) = 4\). Now we suppose that \(S_m\) is isomorphic to \(W_6\). \(W_6\) have spectrum \{-2, -1, 0, 0, 1, 2\} and 6 vertices. Thus, \(E(W_6) = 6\). Hence, the result follows. □

**Theorem 2.7** Let \(S_m\) be smith graph and \(E(S_m)\) be its energy. Then \(E(S_m) = (m + 1)\) if and only if \(S_m\) is isomorphic to either \(C_3\) or \(H_7\).

**Proof.** The necessity part of the proof can be given by the same argument as given in proof of Theorem 2.6 For the sufficiency part, let us assume that \(S_m\) is isomorphic to \(C_3\). Clearly, \(C_3\) have 3 vertices and its spectrum is \{-1, 1, 2\}. Thus, \(E(C_3) = 4 = m + 1\). Next let us take \(S_m\) to be \(H_7\), which has 7 vertices and spectrum is \{-1, 1, 2, 0, 1, 1, 2\}. Therefore, \(E(H_7) = 8 = (m + 1)\). Hence, the result. □

**Theorem 2.8** Let \(S_1\) and \(S_2\) be two smith graphs having vertices set \(V(S_1)\) and \(V(S_2)\), respectively such that \(|V(S_1)| < |V(S_2)|\). Then, \(E(S_1) \leq E((S_2))\).

**Proof.** In order to show the result, we shall pick up those smith graphs \(S_1\) and \(S_2\) for which \(|V(S_1)| < |V(S_2)|\). First, we consider \(C_3\) whose spectrum is \{1, 1, 2\}. Therefore, \(E(C_3) = 4\). We need to tackle the following cases:

Case (i) Let \(S_2 \cong C_4\). In light of Lemma 2.1, \(E(C_4) = 4\). Therefore \(E(C_3) = E(C_4)\).

Case (ii) Let us take \(S_2 \cong K_{1,4}\). Then, clearly \(E(K_{1,4}) = 4\). Therefore \(E(C_3) = E(K_{1,4})\).

Case (iii) Let \(S_2 \cong H_7\) or \(H_8\) or \(H_9\). Then, in view of Lemma 2.1, we see that energy of each of the listed graphs is greater than \(E(C_3)\).

Case (iv) Let us assume \(S_2 \cong W_m\) \((m \geq 6)\). Due to Lemma 2.1, we get \(E(W_m) > E(C_3)\).

Case (v) When we assume \(S_2 \cong C_m\) \((m > 4)\). Clearly, the strict inequality holds between the energy of \(S_1\) and \(S_2\).

Next if we choose \(S_1\) and \(S_2\) to be any of the smith graph namely \(K_{1,4}\), \(H_7\), \(H_8\), \(H_9\), \(W_m\) and \(C_m\) in such a way that \(|V(S_1)| < |V(S_2)|\), then we can easily prove the result for each case by following the same technique. Thus, for any two smith graph having \(|V(S_1)| < |V(S_2)|\), we have \(E(S_1) \leq E((S_2))\). □

**Remark 2.9** If two smith graphs have equal number of vertices, then their energies need not be same. As for instance, consider \(C_5\) and \(K_{1,4}\). Both the graphs have same number of vertices. However, the energy of \(C_5\) is 6.47 and the energy of \(K_{1,4}\) is 4, which are not equal.

**Remark 2.10** The minimum energy of smith graph is 4. Moreover, the minimum energy is attained by more than one smith graphs. The graphs \(C_3\), \(C_4\)
and $K_{1,4}$ all have the same energy.

**Theorem 2.11** Among all the smith graphs $K_{1,4}$ is the only smith graph which is hypoenergetic.

**Proof.** In order to show the result $E(K_{1,4}) < m$ and for all other smith graph $E(S_m) \geq m$.

If we take $S_m$ to be $C_6$ then by Theorem 2.5., $E(C_6) = m + \left\lceil \frac{n}{3} \right\rceil > m$.

Therefore, $C_6$ is non-hypoenergetic.

Let us assume $S_m$ to be either $C_4$ or $W_6$ then by Theorem 2.6., $E(C_4) = 4$ and $E(W_6) = 6$. Hence $C_4$ and $W_6$ are non-hypoenergetic.

Let us take $S_m$ to be either $C_3$ or $H_7$ then by Theorem 2.7. $E(S_m) = (m+1) > m$. Therefore, $C_3$ and $H_7$ are non-hypoenergetic.

If we take $S_m$ be $W_m(m \geq 7)$, $C_m(m \neq 3, 4, 6)$, $H_8$ and $H_9$. In view of Theorem 2.2., $(m-1) < E(S_m) < m + \left\lceil \frac{n}{3} \right\rceil$. Thus all listed smith graph is non-hypoenergetic.

Let we take $S_m$ to be $K_{1,4}$ then by Theorem 2.4, $E(K_{1,4}) = 4$. Therefore, $E(S_m) = (m-1) < m$. Hence $K_{1,4}$ is a hypoenergetic. From the forgoing analysis, we found that the only hypoenergetic graph is $K_{1,4}$. \qed

**Remark 2.12** Following are non co-spectral equienegetic graphs

- $C_3$, $C_4$ and $K_{1,4}$
- $C_3$, $C_4$ and $C_6$
- $C_3$, $C_4$ and $H_7$

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