SOME RELATIONS BETWEEN RANK, CHROMATIC NUMBER AND ENERGY OF GRAPHS

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Abstract

The energy of a graph $G$ is defined as the sum of the absolute values of all eigenvalues of $G$ and denoted by $E(G)$. Let $G$ be a graph and $\text{rank}(G)$ be the rank of the adjacency matrix of $G$. In this paper we characterize all the graphs with $E(G) = \text{rank}(G)$. Among other results we show that apart from a few families of graphs, $E(G) \geq 2\max(\chi(G), n - \chi(\Gamma))$, where $\Gamma$ and $\chi(G)$ are the complement and the chromatic number of $G$, respectively. Moreover some new lower bounds for $E(G)$ in terms of $\text{rank}(G)$ are given.
Introduction

Let $G$ be a graph. Throughout this paper the order of $G$ is the number of vertices of $G$. In this paper all of the graphs that we consider are finite, simple and undirected. If $\{v_1, \ldots, v_n\}$ is the set of vertices of $G$, then the adjacency matrix of $G$, $A = [a_{ij}]$, is an $n \times n$ matrix whose entries $a_{ij}$ is given by $a_{ij} = 1$, if $v_i$ and $v_j$ vertices are adjacent and $a_{ij} = 0$ otherwise. Thus $A$ is a symmetric matrix with zeros on the diagonal, and all eigenvalues of $A$ are real. We know that $\text{rank}(A)$ is equal to the number of non-zero eigenvalues of $G$. For a graph $G$, $\text{rank}(G)$, denotes the rank of the adjacency matrix of $G$. The spectrum of graph $G$, $\text{Spec}(G)$, is the set of real numbers which are the eigenvalues of $A$, together with their multiplicity. We denote the path and the complete graph of order $n$ by $P_n$ and $K_n$, respectively. The complete $t$-partite graph is a graph whose vertices can be partitioned into $t$ subsets so that two vertices are adjacent if and only if they belong to different subsets of the partition. We denote the complete bipartite graph by $K_{r,s}$. A matching of $G$ is a set of mutually non-incident edges. A perfect matching of $G$ is a matching which covers all vertices of $G$. For the graph $G$, the chromatic number of $G$, $\chi(G)$, is the minimum number of colors needed to color the vertices of a graph such that no two adjacent vertices have the same color.

The Huckel molecular orbital, HMO theory, is nowadays the most important field of theoretical chemistry where graph eigenvalues occur. HMO theory deals with unsaturated conjugated molecules, that only $\pi$-electrons are interested in it. The vertices of the graph associated with a given molecule are in one to one correspondence with the carbon atoms of the hydrocarbon system. Two vertices in the graph are adjacent if and only if there is a $\sigma$-electron bond between the corresponding carbon atoms. Calculation of the totally energy of $\pi$-electron in conjugated hydrocarbons can be reduced to $\sum_{i=1}^{n} |\lambda_i|$ in which $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of matrix $A$, where $A$ is the adjacency matrix of the associated graph. The energy of a graph $G$ is defined the sum of the absolute values of all eigenvalues and denoted by $E(G)$. If $\lambda_1, \ldots, \lambda_n$ are all positive eigenvalues of a graph $G$, then we have $E(G) = 2(\lambda_1 + \cdots + \lambda_n) = -2(\lambda_{n+1} + \cdots + \lambda_n)$, since $tr(A) = 0$. For a survey on the energy of graphs, see [12].

First we begin with the following simple lemma.

Lemma 1. [6, p. 21] If for every eigenvalue $\lambda$ of a graph $G$, $\lambda \geq -1$, then $G$ is the union of complete graphs.

In [7], it is shown that for any graph $G$, $E(G) \geq \text{rank}(G)$. Here we characterize all graphs $G$ for which $E(G) = \text{rank}(G)$.

Lemma 2. Let $G$ be a graph of order $n$. Then $E(G) \geq \text{rank}(G)$ and the equality holds if and only if $G = \frac{r}{2}K_2 \cup (n - r)K_1$, for some positive integer $r$. 
**Proof.** Assume that $\lambda_1, \ldots, \lambda_r$ are all non-zero eigenvalues of $G$. Let $\lambda^n - (\lambda^r + a_1\lambda^{r-1} + \cdots + a_r)$ be the characteristic polynomial of $G$, where $a_r$ is a nonzero integer. Then the arithmetic-geometric inequality implies that

$$\frac{\sum |\lambda_i|}{r} \geq \sqrt[2]{\prod |\lambda_i|} \geq \sqrt[2]{|a_r|} \geq 1. \tag{1}$$

Thus $E(G) \geq \text{rank}(G)$. If $G = \frac{r}{2}K_2 \cup (n - r)K_1$, obviously $E(G) = \text{rank}(G)$. Conversely, suppose that $E(G) = \text{rank}(G)$. So the equality holds in (1), that is $|\lambda_1| = \cdots = |\lambda_r| = 1$. Now, by Lemma 1, $G = \frac{r}{2}K_2 \cup (n - r)K_1$. \hfill $\square$

**Remark 1.** In [3], it is shown that if the energy of a graph is rational, then it must be an even integer. Here, we give a simple proof for this result. To prove first we note that the sum of algebraic integers is an algebraic integer. Since $\sum_{\lambda \in \text{Spec}(G)} \lambda = 0$, $E(G)/2$ is equal to the sum of positive eigenvalue of $G$. So $E(G)/2$ is an algebraic integer. Now if $E(G)$ is rational, then $E(G)/2$ should be an integer.

In [2], it is shown that the energy of a connected graph is greater than 1. In the following we improve this lower bound.

**Theorem 1.** For any connected graph $G$ apart from $K_1$ and $K_{1,i}, 1 \leq i \leq 3$, $E(G) \geq 4$.

**Proof.** We may assume that $G$ has at least four vertices. Clearly, rank($G$) $\geq 2$. If rank($G$) = 2, it is well-known that (cf. [1]) $G$ is a complete bipartite graph. So $G$ is $K_{r,s}$ and $rs \geq 4$. So $E(G) \geq 2\sqrt{rs} \geq 4$. If rank($G$) = 3, then $G$ is a complete 3-partite graph, see Table 1 in [1]. Therefore $G$ has $K_3$ as an induced subgraph. Thus by Interlacing Theorem (Theorem 0.10 of [6]) $E(G) \geq E(K_3) = 4$. If rank($G$) $\geq 4$, then by Lemma 2, $E(G) \geq 4$. \hfill $\square$

**Theorem 2.** Let $G$ be a connected bipartite graph and rank($G$) = $r$, then $E(G) \geq \sqrt{(r + 1)^2 - 5}$.

**Proof.** Let $\lambda_1, \ldots, \lambda_{r/2}$ be the positive eigenvalues of $G$. Then

$$E(G)^2 = (2\sum_{i=1}^{r/2} \lambda_i)^2 = 4(\sum_{i=1}^{r/2} \lambda_i^2 + \sum_{i \neq j} \lambda_i \lambda_j) = 4(m + \frac{r}{2}(\frac{r}{2} - 1)a),$$

where $a$ is the arithmetic mean of $\{\lambda_i \lambda_j\}_{i \neq j}$. The geometric mean of $\{\lambda_i \lambda_j\}_{i \neq j}$ is

$$\prod_{i \neq j} \lambda_i \lambda_j)^{\frac{1}{r}(\frac{r}{2} - 1)} = k^{2/r},$$

where $k = \lambda_1^2 \cdots \lambda_{r/2}^2$. Since $G$ is connected, $m \geq r - 1$, where $m$ is the number of edges of $G$. We have $k \geq 1$, so we find
Lemma 3. If $F$ is a forest with no perfect matching and isolated vertex, then $F$ has at least two maximum matchings.

Proof. It is sufficient to show that $F$ has a maximum matching which does not saturate a pendent vertex. Let $|V(F)| = n$. We apply induction on $n$. Clearly the assertion is true for $n = 3$. Consider a forest $F$ of order $n$ with $n > 3$. Let $v_1$ be a pendent vertex adjacent to $v_2$ and $M$ be a maximum matching for $F$. If $v_1v_2 \notin M$ we are done. If $v_1v_2 \in M$, then consider the forest $F \setminus \{v_1, v_2\}$. If $F \setminus \{v_1, v_2\}$ has an isolated vertex, then we are done. If $F \setminus \{v_1, v_2\}$ has no isolated vertices, by induction hypothesis we obtain a maximum matching of $F \setminus \{v_1, v_2\}$, say $M'$ which does not saturate a pendent vertex $v_i$. If $v_i$ is not adjacent to $v_2$, then $M' \cup \{v_1v_2\}$ is the desired maximum matching of $F$, while if vertex $v_i$ is adjacent to $v_2$, the $M' \setminus \{e\} \cup \{v_2v_i\}$, where $e \in M'$ and $e$ is incident with $v_i$, is the desired maximum matching.

The following lemma is an immediate consequence of Harary’s Theorem, see [4, p.44].

Lemma 4. The number of maximum matching of a tree is equal to the product of its non-zero eigenvalues.

Corollary 1. Let $G$ be a bipartite graph with at least 4 vertices. If $G$ is not full rank, then $E(G) \geq 1 + \text{rank}(G)$.

Proof. With no loss of generality we may assume that $G$ is a connected graph. By the proof of Theorem 2, we have $E(G) \geq \sqrt{4m + r(r - 2)k^2}$, where $r = \text{rank}(G)$ and $k = \lambda_1^2 \cdots \lambda_{r/2}^2$ and $\lambda_1, \ldots, \lambda_{r/2}$ are non zero eigenvalues of $G$. If $G$ is a tree, then by Theorem 8.1 of [6, p. 233], $G$ has no perfect matching. Thus Lemmas 3 and 4 imply that $k \geq 4$. Thus $E(G) \geq \sqrt{4r + r(r - 2)\sqrt{4}}$. If $r \geq 3$, then $(\sqrt{4} - 1)r^2 + 2r(1 - \sqrt{4}) - 1 \geq 0$, since

$$r^2 - 2r \geq \frac{r\sqrt{4r^2 - 1}}{3} \geq \frac{\sqrt{4r^2 - 1} + \sqrt{4r^2 - 4} + \cdots + 1}{3}.$$

Therefore $E(G) \geq r + 1$. If $r = 2$, by Theorem 1 we are done. If $G$ is not a tree, then $m \geq r + 1$ and the proof is complete.

Now we would like to obtain some lower bounds for $E(G)$ in terms of chromatic number of $G$ and chromatic number of $\overline{G}$. 

\[ E(G) \geq \sqrt{4m + r(r - 2)k^2} \geq \sqrt{(r + 1)^2} - 5. \]
Theorem 3. For any connected graph \( G \), \( E(G) \geq 2(n - \chi(G)) \).

Proof. By Theorem 2.30 of [8], \( n - \chi(G) \leq \lambda_1 + \cdots + \lambda_{\chi(G)} \). Thus \( E(G) \geq 2(n - \chi(G)) \). \( \square \)

Remark 2. A well-known theorem of Nordhaus and Gaddum [13] states that for every graph \( G \) of order \( n \), \( \chi(G) + \chi(\overline{G}) \leq n + 1 \). The graphs attaining equality in the Nordhaus-Gaddum Theorem were characterized by Finck [9], who proved that there are exactly two types of such graphs, the types (a) and (b) defined as follows.

(i) A graph \( G \) has type (a) if it has a vertex \( v \) such that \( V \setminus \{v\} \) can be partitioned into subsets \( K \) and \( S \) with the properties that \( K \cup \{v\} \) induces a clique of \( G \) and \( S \cup \{v\} \) induces an independent set of \( G \) (adjacency between \( K \) and \( S \) is arbitrary). Note that if \( G \) has type (a), then so does its complementary graph \( \overline{G} \).

(ii) A graph \( G \) has type (b) if it has a subset \( C \) of five vertices such that \( V \setminus C \) can be partitioned into subsets \( K \) and \( S \) with the properties that \( K \) induces a clique, \( S \) induces an independent set, \( C \) induces a 5-cycle, and every vertex of \( C \) is adjacent to every vertex of \( K \) and to no vertex of \( S \) (adjacency between \( K \) and \( S \) is arbitrary). Note that if \( G \) has type (b), then so does its complementary graph.

If we omit a perfect matching from the complete graph \( K_{2n} \), the resulting graph called cocktail party and denoted by \( CP(n) \). A generalized line graph \( L(G;a_1,\ldots,a_n) \) is defined for graphs with \( n \) vertices \( \{1,\ldots,n\} \) and nonnegative integers \( a_1,\ldots,a_n \) by taking the graph \( L(G) \) and \( CP(a_i) \) and adding extra edges. A vertex in \( L(G) \) is joined to one in \( CP(a_i), i = 1,\ldots,n \), if vertex \( i \) is an end point of the vertex in \( L(G) \)(viewed as an edge of \( G \)).

We denote by \( A_{n,t} \), \( 1 \leq t \leq n \), the graph obtained by joining a vertex to \( t \) vertices of the complete graph \( K_n \). If we add two pendant vertices to a common vertex of \( K_n \), the resulting graph has order \( n + 2 \) and we denote it by \( B_n \). For the proof of the next theorem we need the following interesting result due to Wilf, see [4, p.55].

Lemma 5. For any graph \( G \), \( \chi(G) \leq \lambda_1(G) + 1 \).

Theorem 4. Let \( G \) be a graph. Then \( E(G) < 2\chi(G) \) if and only if \( G \) is a union of some isolated vertices and one of the following graphs:

(i) the complete graphs \( K_n \);
(ii) the graphs \( B_n \);
(iii) the graphs \( A_{n,t} \) for \( n \leq 7 \), beside \( (n,t) = (7,4) \), and for \( n \geq 8 \) with \( t \in \{1,2,n-1\} \);
(iv) a triangle with two pendant edges adjacent to different vertices (graph \( H_5 \)).
Proof. If \( G \) has two non-trivial component, then \( G \) has \( 2K_2 \) as an induced subgraphs. Now by Interlacing Theorem (Theorem 0.10 of [6]) and Lemma 5 we find that \( E(G) \geq 2(\lambda_1 + \lambda_2) \geq 2(\lambda_1 + 1) \geq 2\chi(G) \). Since isolated vertices does not effect on the energy and the chromatic number, we may assume that \( G \) is connected. by Remark 2 we have \( \chi(G) + \chi(\overline{G}) \leq n + 1 \). Now we consider two cases:

Case 1. \( \chi(G) + \chi(\overline{G}) \leq n \). In this case \( \chi(G) \leq n - \chi(\overline{G}) \), and by Theorem 3, are done.

Case 2. \( \chi(G) + \chi(\overline{G}) = n + 1 \). In this case \( G \) has type \( a \) or type \( b \). If \( G \) has type \( b \), then \( G \) has \( C_5 \) as an induced subgraph. Therefore we find that \( \lambda_2 + \lambda_3 \geq \lambda_2(C_5) + \lambda_3(C_5) > 1 \). Thus by Lemma 5 we have

\[
E(G) \geq 2(\lambda_1 + \lambda_2 + \lambda_3) > 2(1 + \lambda_1) \geq 2\chi(G).
\]

Thus one may assume that \( G \) has type \( a \). For simplification let \( |K| = t \), where \( K \) is a complete subgraph of \( G \) defined in remark 2. It is easily seen that \( \chi(G) = t + 1 \). Clearly, \( K_{t+1} \) is an induced subgraph of \( G \).

We know that \( \mu_1 = t \), \( \mu_2 = \cdots = \mu_{t+1} = -1 \) are eigenvalues of \( K_{t+1} \). So by Interlacing Theorem, \( G \) has at least \( t \) eigenvalues which are at most \(-1\). If \( G \) has an induced subgraph with at least one eigenvalue \( \lambda \) such that \( \lambda \leq -2 \), then the sum of all negative eigenvalues of \( G \) is less than \(-t - 2 = t - 1 \). Since the sum of all eigenvalues of \( G \) is zero, if \( \lambda_1, \ldots, \lambda_s \) are all positive eigenvalues of \( G \), then \( \lambda_1 + \cdots + \lambda_s \geq t + 1 \). Thus \( E(G) = 2(\lambda_1 + \cdots + \lambda_s) \geq 2t + 2 = 2\chi(G) \).

Therefore we may assume that every eigenvalue of each induce subgraph of \( G \) is more than \(-2 \). This implies that \( G \) has no \( K_{1,4} \) as an induced subgraph. This yields that every vertex of \( K \) is adjacent to at most two vertices of \( S \). First suppose that there is a vertex \( a \in K \) which is adjacent to two vertices \( \{x, y\} \subseteq S \).

Let \( |S| \geq 3 \). Thus there exists a vertex \( z \in S\setminus\{x, y\} \) such that \( z \) is adjacent to a vertex \( b \in K \) and \( b \neq a, v \). Thus \( G \) has either \( H_1 \), or \( H_2 \) as an induced subgraph.

![Diagram of graphs H1 and H2](image)

Since \( \lambda_6(H_1) < -1.8 \), \( \lambda_5(H_1) < -1.3 \), and \( \lambda_6(H_2) < -1.7 \), \( \lambda_6(H_2) < -1.6 \), see [14], as before we conclude that \( E(G) \geq 2\chi(G) \). Thus in this case we can assume that \( G = B_{n-2} \).

Now, suppose that every vertex in \( K \) is adjacent to at most one vertex of \( S \). If \( |S| \geq 2 \) and \( |K| \geq 3 \) then \( G \) has an induced subgraph isomorphic to \( H_3 \) or \( H_4 \).
But $H_3$ has two eigenvalues which one of them is less than $-1.39$ and another one is less than $-1.61$. Also $H_4$ has two eigenvalues which one of them is less than $-1.3$ and another less than $-1.7$, see [14]. Thus $E(G) \geq 2\chi(G)$. This implies that $|S| \leq 1$ or $|K| \leq 2$. If $|S| = 0$, then $G = K_n$. If $|S| = 1$, then $G = A_{n,t}$ for some $t$.

If $|K| \leq 2$, then $|S| \leq 2$. It can be easily checked that $G$ isomorphic to $B_1(\simeq K_{1,2})$, $A_{3,1}$, $A_{3,2}$, $H_5$ or $K_i$, $i = 1, 2, 3$.

The characteristic polynomial of $B_n$ (see [6, p. 159]) is

$$
\lambda(\lambda + 1)^{n-2}((\lambda^2 - 2)(\lambda - n + 2) + \lambda(\lambda - n + 1)(\lambda + 1) + \lambda^2(\lambda - n + 2)).
$$

Therefore $B_n$ has at least $n-2$ eigenvalues $-1$. By Lemma 1 and Theorem 6.7 of [6], $\lambda_{n+2} < -1$ and so $B_n$ has exactly two positive eigenvalues. This implies that $E(B_n) = -2(\lambda_{n+2} - n + 2)$. On the other hand the characteristic polynomial of $B_n$ is $\lambda(\lambda + 1)^{n-2}f(\lambda)$, where $f(\lambda) = \lambda^3 + (2 - n)\lambda^2 - (1 + n)\lambda + 2n - 4$. So $f'(\lambda) = 3\lambda^2 + (4 - 2n)\lambda - n - 1$ and $f''(\lambda) = 6\lambda + 4 - 2n$. If $\lambda \leq -2$ then $f''(\lambda) < 0$ so $f'(\lambda) > f'(-2) > 0$. So $f(\lambda) < f(-2) = -2$. Therefore all eigenvalues of $B_n$ are more than $-2$. Thus $E(B_n) = -2(\lambda_{n+2} - n + 2) < 2n$.

A calculation shows that for $n \leq 7$, $E(A_{n,t}) < 2n$ except $E(A_{7,4}) = 14$. So we let $n \geq 8$. The graph $K_n$ has $n-1$ eigenvalues $-1$, therefore by Interlacing Theorem, the graph $A_{n,t}$ has at least $n-2$ eigenvalues $-1$. On the other hand the graphs $A_{n,1}$ and $A_{n,2}$ are not complete multipartite graphs so they have at least two positive eigenvalues. Then again Interlacing Theorem implies that these two graph have exactly two positive eigenvalues. The graphs $A_{n,1}$ and $A_{n,2}$ are line graphs, and $A_{n,n-1} = L(K_{1,n-1}; 1, 0, \ldots, 0)$, where the vertex with index $1$ in $K_{1,n}$ is the vertex with maximum degree. Hence their eigenvalues are at least $-2$ and Theorem 1.6 of [5] shows that $\lambda_{n+1} > -2$. Thus $E(A_{n,t}) = -2(\lambda_{n+1} - n + 2) < 2n$. The graph $A_{n,n-1}$ has a zero eigenvalue, and in the same way we find that $E(A_{n,n-1}) < 2n$. Now let $2 < t < n - 1$. In this circumstance, the graph $A_{n,t}$ cannot be a generalized line graph, thus by Exercise 14 of [11, p. 278], $\lambda_{n+1} \leq -2$. Hence $E(A_{n,t}) \geq 2n$. □
Let $G$ be a connected graph of order $n$. The following corollary shows that either the graph $G$, or $\overline{G}$ has energy at least $n$. Compare with Corollary 5.2 of [12] which states that if $G$ has no zero eigenvalue, then $E(G) \geq n$.

**Corollary 2.** For any connected graph $G$ of order $n \geq 3$, apart from complete graphs, the graphs $A_{k,k-1}$, $B_1$, $B_2$, and $A_{3,1}$, $E(G) + E(\overline{G}) \geq 2n$.

**Proof.** If $\overline{G}$ is not one of the graphs described in Theorem 4, we are done. If $G$ is a complete graph, $B_1$, $B_2$, or $A_{3,1}$, it is easily seen that $E(G) + E(\overline{G}) < 2n$. If $G \simeq A_{k,k-1}$, then $E(G) + E(\overline{G}) < 2k + 2 = 2n$. To complete the proof, it is enough to show that theorem holds for $B_k$, $k \geq 3$ and $A_{k,t}$ for $k \geq 4$, and $t = 1, 2$. The graph $B_k$ has $k-2$ eigenvalue $-1$, and $\lambda_n(B_k) \leq \lambda_6(B_k) < -1.8$. So $E(B_k) > 2(k - 0.2)$. On the other hand $K_{1,1,2}$ is an induced subgraph of $B_k$. Therefore $E(B_k) \geq E(K_{1,1,2}) > 5$ and so $E(B_k) + E(\overline{B_k}) \geq 2k + 2$.

The graph $A_{k,t}$ has $k-1$ eigenvalue $-1$ and $\lambda_n(A_{k,1}) \leq \lambda_5(A_{4,1}) < -1.5$, so $E(A_{k,1}) > 2k - 1$. Also $\lambda_n(A_{k,2}) \leq \lambda_5(A_{4,2}) < -1.68$, hence $E(A_{k,1}) > 2k - 0.64$. Since $E(A_{k,1}) \geq E(K_{1,3}) > 3.4$, $E(A_{k,2}) \geq E(K_{1,2}) > 2.8$ and he proof is complete. □

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