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On the Energy of Singular and Non Singular Graphs

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Abstract

Let G be a simple undirected graph with n vertices, m edges, adjacency matrix A, largest eigenvalue ρ and nullity κ. The energy of G, $\mathcal{E}(G)$ is the sum of its singular values. In this work lower bounds for $\mathcal{E}(G)$ in terms of the coefficient of μ^{κ} in the expansion of characteristic polynomial, $p(\mu) = \det(\mu I - A)$ are obtained. In particular one of the bounds generalizes a lower bound obtained by K. Das, S. A. Mojallal and I. Gutman in 2013 to the case of graphs with given nullity. The bipartite case is also studied obtaining in this case, a sufficient condition to improve the spectral lower bound 2ρ. Considering an increasing sequence convergent to ρ a convergent increasing sequence of lower bounds for the energy of G is constructed.

1 Preliminaries

This work deals with an (n, m)-graph G which is an undirected simple graph with vertex and edge set $V(G)$ and $E(G)$ with cardinality n and m, respectively. A *matching,* say

W, in G is a subset of $E(G)$ such that any pair of edges in W does not share any vertex. A *perfect matching* W is a matching W such that its set of vertices coincides to $V(G)$. For $i \in V(G)$ the set $N_G(i) = \{j \in V(G) : ij \in E(G)\}$ is called *the neighborhood of the vertex* i and its cardinality is the *vertex degree* i. The vertex degree i is denoted by $d(i), \quad \forall 1 \le i \le n$. As usual, the complete graph, the cycle, with n vertices and the complete bipartite graph with bipartition (X, Y) are denoted by K_n, C_n and $K_{x,y}$, respectively, where the cardinality of X and Y are x and y. The adjacency matrix, $A(G)$, is simply denoted by A. The number of walks of length k of G starting at i corresponds to the i-th row sum of A^k, is referred as *the vertex k-degree* i and it is denoted by $d_k(i)$ (see [9]). For convenience, we set

$$d_0(i) = 1, \; d_1(i) = d(i), \text{ and}$$
$$d_{k+1}(i) = \sum_{j \in N_G(i)} d_k(j), \quad \forall k \ge 1.$$

A graph G with n vertices is called a *regular* graph (or s-*regular*) if $d(i) = s, \quad \forall\, 1 \le i \le n$. Note that if $\mathbf{v}_k = (d_k(1), \ldots, d_k(n))^T$, then $\mathbf{v}_0 = \mathbf{e}$, the n-dimensional all ones vector and $\mathbf{v}_{k+1} = A\mathbf{v}_k, \quad \forall k \ge 0$. Moreover, if G is s-regular, then $\mathbf{v}_k = s^k \mathbf{e}$ and

$$s = \sqrt{\frac{\mathbf{v}_{k+2}^T \mathbf{v}_{k+2}}{\mathbf{v}_k^T \mathbf{v}_k}}, \quad \forall k \ge 0.$$

We establish now some facts from Matrix Theory used throughout the text. During the paper R and M stands for a Hermitian complex and an arbitrary complex matrix, respectively, both of order n. The *energy* of the Hermitian matrix R, denoted by $\mathcal{E}(R)$, is the sum of its singular values that is, the sum of the absolute values of its eigenvalues. The *nullity* of M, denoted by $\eta(M)$, corresponds to the multiplicity of the null eigenvalue of M^*M, where M^* is the conjugate transpose matrix of M. Thus, M is nonsingular ($\det M \neq 0$) if and only if $\eta(M) = 0$. The *rank* of a square matrix M of order n is $r(M) = n - \eta(M)$, see [17]. On the other hand, the *k-th elementary symmetric sum* of the eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$ of a square matrix M of order n, see [17], is defined as

$$\Upsilon_k(M) = \sum_{1 \le i_1 < i_2 < \cdots < i_k \le n} \mu_{i_1} \mu_{i_2} \cdots \mu_{i_k}, \quad \forall 1 \le k \le n. \tag{1}$$

Note that $\Upsilon_n(M) = \det(M)$ and $\Upsilon_1(M) = \mathrm{tr(M)}$, with $\det(.)$ and $\mathrm{tr}(.)$ denoting the determinant and the trace of a square matrix. For a matrix M of order n, let $M[i_1, i_2, \ldots, i_k]$ be the principal submatrix of M whose j-th row and column are labeled by $i_j, \quad \forall 1 \le j \le k$.

Then, $\det(M[i_1, i_2, \ldots, i_k])$ is a *principal minor of order k of M*. At this point we need to write the identity matrix of the order t as I_t, $\quad \forall t \geq 1$, and if the order is clear from the context we simply use I. It follows a known result from linear algebra, (see [17, Ch. 7]).

Lemma 1. *[17] Let M be a matrix of order n and let $q(\mu) = \det(\mu I - M)$, the characteristic polynomial of M. Let*

$$q(\mu) = \mu^n + c_1\mu^{n-1} + c_2\mu^{n-2} + \cdots + c_{n-1}\mu + c_n.$$

If $\Upsilon_k(M)$ is the k-th elementary symmetric sum of the the roots of $q(\mu)$, then

1. $c_k = (-1)^k \sum$ *(all $k \times k$ principal minors)*
2. $\Upsilon_k(M) = \sum$ *(all $k \times k$ principal minors)*

Therefore,

$$|c_k| = |\Upsilon_k(M)| = \left| \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq n} \det(M[i_1, i_2, \ldots, i_k]) \right|. \tag{2}$$

As an immediate consequence, we can write the next remark.

Remark 1. *Let R be a Hermitian matrix of rank $n - \kappa$ whose nonzero eigenvalues are $\alpha_{j_1}, \ldots, \alpha_{j_{n-\kappa}}$, then its characteristic polynomial, say $\overline{q}(\mu)$, can be factorized as*

$$\begin{aligned}\overline{q}(\mu) &= \mu^\kappa \left(\mu^{n-\kappa} + \overline{c}_1\mu^{n-1-\kappa} + \overline{c}_2\mu^{n-2-\kappa} + \cdots + \overline{c}_{n-1}\mu + \overline{c}_{n-\kappa}\right) \\ &= \mu^\kappa (\mu - \alpha_{j_1})(\mu - \alpha_{j_2}) \ldots \left(\mu - \alpha_{j_{n-\kappa}}\right),\end{aligned}$$

where

$$|\overline{c}_{n-\kappa}| = \left|\prod_{l=1}^{n-\kappa} \alpha_{j_l}\right| = |\Upsilon_{n-\kappa}(R)| = \tag{3}$$

$$\left| \sum_{1 \leq i_1 < i_2 < \cdots < i_{n-\kappa} \leq n} \det(R[i_1, i_2, \ldots, i_{n-\kappa}]) \right|. \tag{4}$$

For a graph G, its eigenvalues, say $\lambda_1 \geq \cdots \geq \lambda_n$, are the eigenvalues of A (see e.g. [6,7]). The singular values of G are the square roots of the eigenvalues of A^*A. Since, A is real and symmetric the singular values of G are the absolute values of its eigenvalues. If G is a connected graph, then A is a non-negative symmetric irreducible matrix [6]. The nullity of A is called the *nullity* of G and it is denoted by $\eta(G)$, see [10]. Consequently, a graph

G is called *nonsingular* if $\eta(G) = 0$, otherwise is called *singular*. We simply denote the rank of A, $r(A)$, by r. The paper is organized as follows. At Section 2 some motivation in connection with Chemistry, known lower bounds for $\mathcal{E}(G)$ and three subsections are presented in which the main results are classified. In section 3, by using the increasing sequence of lower bounds for ρ given in [5] an increasing sequence of lower bounds for the energy of graphs with nullity κ, is obtained. Equality cases are studied. Additionally, at Section 4 some tables, comparing the results, are presented.

2 Main results

The notion of energy of a graph arose in Mathematical Chemistry. Important references for this definition and its applications are in [12,15]. For a graph G, the following equality.

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|, \tag{5}$$

is called the *energy* of the graph G, ([11]). The search for upper bounds for this graph invariant has been intense, see ([15]). Concerning lower bounds for the energy of a graph the reader should be referred, for instance, to [2, 3, 16, 19]. For a non-singular connected (n, m)-graph in [8], Das et al. obtained the following lower bound for $\mathcal{E}(G)$

$$\mathcal{E}(G) \geq \frac{2m}{n} + (n-1) + \ln|\det A| - \ln\frac{2m}{n}. \tag{6}$$

Note that if $\det A = 0$, this lower bound can not be applied. The equality holds in (6) if and only if G is the complete graph K_n. The last lower bound was obtained firstly considering that, for a connected graph, the following relationship holds.

$$\mathcal{E}(G) \geq \rho + (n-1) + \ln|\det A| - \ln\rho. \tag{7}$$

In [8] it was shown that the graph that attains equality in (7) is the same graph that attains equality in (6).

A spectral lower bound for the energy can be seen in [4],

$$\mathcal{E}(G) \geq 2\rho, \tag{8}$$

where, if G is connected, the equality holds in (8), for example, if G is a complete graph and a complete bipartite graph.

The following simple lower bound for a graph G with m edges was introduced by Caporossi et al. in [4] and the equality case was discussed. In fact,

$$\mathcal{E}(G) \geq 2\sqrt{m}, \tag{9}$$

with equality if and only if G consists of a complete bipartite graph $K_{a,b}$ such that $ab = m$ and arbitrarily many isolated vertices. In [1] the following lower bounds for $\mathcal{E}(G)$ were introduced.

1. For an (n, m)-graph G without isolated vertices, with nullity $\eta(G) = \kappa = n - r$, where $0 \leq \kappa \leq n - 1$ $(1 \leq r \leq n)$,

$$\mathcal{E}(G) \geq \frac{\sqrt{8m + 4r(r-1)\left|\Upsilon_r(G)\right|^{\frac{2}{r}}}}{2}. \tag{10}$$

2. For an (n, m) bipartite graph G without isolated vertices, with nullity $\eta(G) = \kappa = n - r$, where $0 \leq \kappa \leq n - 1$ $(1 \leq r \leq n)$,

$$\mathcal{E}(G) \geq \frac{\sqrt{16m + 4r(r-2)\left|\Upsilon_r(G)\right|^{\frac{2}{r}}}}{2}. \tag{11}$$

In both cases equality holds if and only if all the nonzero eigenvalues of G have the same absolute value. In other words, if and only if $G = \cup_{j=1}^{\ell} K_{a_j,b_j}$, with $a_j b_j = a_i b_i$, for $i \neq j$, $\ell = \frac{n-\kappa}{2}$ and $n = \sum_{j=1}^{\ell}(a_j + b_j)$. The above lower bounds were obtained as functions of the nullity of the graph G. The graphs obtained in the equality cases become graphs with minimum energy within the family of the (n, m)-graphs without isolated vertices with given nullity $\kappa = n - r$. The main results of this work are presented now.

2.1 Lower bounds for the energy of non-negative symmetric matrices with given nullity

In this subsection we present lower bounds for the energy of non-negative symmetric matrices. Recall that R is a Hermitian matrix. Moreover, if R is a non-negative matrix, then R is symmetric and its spectral radius, $\rho(R)$, and its largest eigenvalue coincide, see [18].

Theorem 2. *Let R be a non null, non-negative symmetric matrix of order n with spectral radius $\rho(R)$ such that $\eta(R) = \kappa$. Then*

$$\mathcal{E}(R) \geq \rho(R) + (n - \kappa - 1) + \ln\left|\Upsilon_{n-\kappa}(R)\right| + \ln\rho(R)^{-1}. \tag{12}$$

The equality holds in (12) if and only if the nonzero eigenvalues of R have all modulus equal to 1, except maybe for its largest eigenvalue. In consequence, the inequality (12) is strict if R has null trace and a submatrix of order 3, say R_1, where either

1. $R_1 = \begin{pmatrix} 0 & a & 0 \\ a & 0 & b \\ 0 & b & 0 \end{pmatrix}$ *with* $\sqrt{a^2+b^2} > 1$, *or*

2. $R_1 = \begin{pmatrix} 0 & a & c \\ a & 0 & b \\ c & b & 0 \end{pmatrix}$ *with a vector* $(\alpha, \beta, \gamma)^T$ *such that*

$$\frac{2(a\alpha\beta + b\beta\gamma + c\alpha\gamma)}{\sqrt{\alpha^2+\beta^2+\gamma^2}} < -1.$$

Proof. Let $\alpha_{j_1} \geq \alpha_{j_2} \geq \cdots \geq \alpha_{j_{n-\kappa}}$, with $\alpha_{j_1} = \rho$, be the non-zero eigenvalues of R. In [8] it was proved that

$$x \geq 1 + \ln x, \quad \forall x > 0. \tag{13}$$

Note that the equality holds in (13) if and only $x = 1$. Using the above result, we get

$$\begin{aligned} \mathcal{E}(R) &= \rho + \sum_{j=2}^{n-\kappa} |\alpha_{i_j}| \\ &\geq \rho + n - \kappa - 1 + \sum_{j=2}^{n-\kappa} \ln |\alpha_{i_j}| \\ &= \rho + n - \kappa - 1 + \ln \left| \prod_{j=2}^{n-\kappa} \alpha_{i_j} \right| \\ &= \rho + n - \kappa - 1 + \ln |\Upsilon_{n-\kappa}(R)| - \ln \rho, \end{aligned}$$

where the equality holds if and only if

$$1 = |\alpha_{j_2}| = |\alpha_{j_3}| = \cdots = |\alpha_{j_{n-\kappa}}|.$$

Now we discuss the case when the inequality (12) is strict. If R is non-negative, non null and with null trace then its smallest eigenvalue, say α, is negative. Therefore the sufficient conditions 1. and 2., are obtained from the interlacing of eigenvalues considering the smallest eigenvalues of R and R_1, respectively (see, for instance [13, Corollary 2.2]). In fact, as the smallest eigenvalue of R_1 in 1. is $-\sqrt{a^2+b^2}$ and imposing that this eigenvalue is smaller than -1 (note that, in this case its modulus is greater than 1 and therefore R doesn't fulfill the equality condition as $\sqrt{a^2+b^2} > 1 > -\alpha = |\alpha|$). Thus, the sufficient condition in 1. is obtained. The condition in 2. is obtained from the Rayleigh quotient and the fact that the smallest eigenvalue of a symmetric matrix is at most a Rayleigh quotient of the matrix ([13, 18]). Now, by noticing that either in 1. or in 2. imposing that R has the smallest eigenvalue not equal to -1, using the same argument as before, the sufficient conditions follow. ■

Remark 2. *The coefficient $\Upsilon_{n-\kappa}(R)$ can be obtained by calculating $c_{n-\kappa}$, the coefficient of μ^κ of the characteristic polynomial of R, $\overline{q}(\mu)$, with the formula in (3) which uses the principal minors of order $n-\kappa$ of R. Then by using the formula in (12) one can approximate the energy of R.*

As a consequence of Theorem 2 the following result can be obtained.

Corollary 3. *Let R be a be a non null, non-negative symmetric matrix of order n with largest eigenvalue $\rho(R)$, $\eta(R) = \kappa$ and such that $\mathbf{x}$ is a vector with the Rayleigh quotient*

$$\phi = \frac{\mathbf{x}^T R\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \geq 1, \tag{14}$$

then

$$\mathcal{E}(R) \geq \phi + (n-\kappa-1) + \ln|\Upsilon_{n-\kappa}(R)| + \ln\phi^{-1}. \tag{15}$$

The equality holds in (15) if and only if $\mathbf{x}$ is an eigenvector of R associated to $\rho(R)$ (or equivalently $\phi = \rho(R)$) and all the nonzero eigenvalues of R have absolute values equal to 1, except maybe for its largest eigenvalue.

Proof. Recall that from the Rayleigh quotient $\rho(R) \geq \frac{\mathbf{x}^T R\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \phi$, with equality if and only if $(\rho(R), \mathbf{x})$ is an eigenpair of R (see e.g. [18]). Taking into account that the real functions $f(x) = x - 1 - \ln x$ and $g(x) = x + n - \kappa + \ln|\Upsilon_{n-\kappa}(R)|$ are strictly increasing functions, for $x \geq 1$, we conclude that the function $h = g \circ f$, where

$$h(x) = x + (n-\kappa-1) + \ln|\Upsilon_{n-\kappa}(R)| - \ln x, \quad \forall x > 0, \tag{16}$$

is strictly increasing for $x \geq 1$. Since,

$$E(R) \geq h(\rho(R)) \geq h\left(\frac{\mathbf{x}^T R\mathbf{x}}{\mathbf{x}^T\mathbf{x}}\right) = h(\phi), \tag{17}$$

the inequality in (15) follows. If equality holds then all the inequalities in (17) become equalities and then by using the equality case in Theorem 2, for all nonzero eigenvalue of R (except maybe $\rho(R)$) say α, we have $|\alpha| = 1$ implying that $\alpha = \pm 1$ and $\rho(R) = \frac{\mathbf{x}^T R\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \phi$, as h is strictly increasing. ■

Remark 3. *If R is partitioned into irreducible blocks with one principal main block, say Q, whose spectral radius is the spectral radius of R, $\rho(R)$ such that $Q\mathbf{y} = \rho(R)\mathbf{y}$, for a non null eigenvector $\mathbf{y}$, then reorganizing the diagonal blocks of R using permutation matrices, if necessary, one can see that either R or a similar to R matrix has an associated eigenvector by blocks, $\mathbf{x} = (\mathbf{y}, \mathbf{0}, \ldots, \mathbf{0})^T$ such that the condition (14) is valid and if all the nonzero eigenvalues of R have absolute values equal to 1, except maybe for its largest eigenvalue, the equality in (15) is also obtained.*

2.2 Lower bounds for the energy of general graphs with given nullity

In this subsection the results for an (n, m)-graph G with nullity κ, are obtained. In order to simplify the notation, sometimes we will set

$$n - \kappa = r, \quad \Upsilon_r\left(A(G)\right) = \Upsilon_r(G) \quad \textit{and}$$
$$\rho(A(G)) = \rho, \quad \forall \textit{ graph } G.$$

Note that, if in Theorem 2 the Hermitian matrix R is replaced by the adjacency matrix of a graph G the inequality (18) in Theorem 4 below is obtained. The result in (12), can be generalized for all graphs, including singular graphs as $\Upsilon_r(G)$ can be obtained by a result in [6, Theorem 1.3] which obtains the coefficients of the characteristic polynomial in terms of the so called "elementary figures".

Theorem 4. *Let G be a graph with n vertices, largest eigenvalue ρ and $\eta(G) = \kappa$. Then*

$$\mathcal{E}(G) \geq \rho + (n - \kappa - 1) + \ln|\Upsilon_{n-\kappa}(G)| + \ln \rho^{-1} \tag{18}$$

The equality holds in (18) if and only if the nonzero eigenvalues of G, except maybe for its largest eigenvalue, have all modulus equal to 1. In consequence, if the largest eigenvalue of G is 1 then the equality holds for $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$. On the contrary, if $\rho > 1$ then the equality holds if and only if $G = K_{n-\ell} \cup \kappa K_1 \cup \lfloor \frac{\ell-\kappa}{2} \rfloor K_2$ with $\kappa \leq \ell \leq n-3$.

Proof. The proof of the inequality follows straightforward from the arguments used in the proof of Theorem 2 replacing the non-negative symmetric matrix R by the adjacency matrix of the graph G. For the equality case, and when $\rho = 1$, by an argument given in [1, Theorem 2] (attending that all the eigenvalues are of equal modulus) any connected component of G has nonzero eigenvalues 1 and -1 implying that they are isolated edges and therefore G is the union of isolated edges and isolated vertices, that is $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$. On the other hand, if $\rho > 1$ then G must have a connected component with at least three vertices and one can see that any induced subgraph with three vertices of this component must be a cycle otherwise it would be a path and then from Theorem 2, $A(G)$ would have a submatrix of the form R_1 as in 1. In consequence, using interlacing, the smallest eigenvalue of G would not be -1. Therefore, if there exists a connected component of G with at least three vertices, it must be a complete graph, and then $G = K_{n-\ell} \cup \kappa K_1 \cup \lfloor \frac{\ell-\kappa}{2} \rfloor K_2$ with $\kappa \leq \ell \leq n-3$. Conversely, it is not difficult to see that for the graphs in the statement the equality holds. ■

Remark 4. *Recalling the equation in (2) one can see that* $|\Upsilon_{n-\kappa}(G)|$ *corresponds to* $|c_{n-\kappa}|$. *Since all the entries of* $A(G)$ *are integers, from item 1. in Lemma 1, and taking into account that it is considered the absolute value of the product of the nonzero eigenvalues of* G*, it follows that the coefficient* $c_{n-\kappa}$ *is a nonzero integer. In consequence,*

$$|\Upsilon_{n-\kappa}(G)| \geq 1, \ \forall \, 0 \leq \kappa \leq n-1. \tag{19}$$

From inequalities (18) and (19), we derive the following result.

Theorem 5. *Let* G *be a graph with* n *vertices with largest eigenvalue* ρ *and* $\eta(G) = \kappa$. *Then*

$$\mathcal{E}(G) \geq \rho + (n-\kappa-1) + \ln \rho^{-1}. \tag{20}$$

The equality holds in (20) if and only if $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$.

Remark 5. *Recalling that a graph* G *is called hypoenergetic if its energy is strictly less than the number of its vertices, (see [15, Ch. 9]) one can see that the inequalities in (13) and in (20) show directly a known result, namely, that if* G *is non-singular (* $\kappa = \eta(G) = 0$*) then* G *is not hypoenergetic, (see [15, Ch. 9]).*

As a consequence of Corollary 3 the following result can be obtained.

Corollary 6. *Let* G *be an* (n,m)*-graph with largest eigenvalue* ρ *and let* G_1 *be an* (n_1,m_1) *component such that* $n_1 \geq 2$, $\frac{2m_1}{n_1} \geq 1$ *and whose largest eigenvalues is equal to* ρ. *Therefore*

$$\mathcal{E}(G) \geq \frac{2m_1}{n_1} + (n-\kappa-1) + \ln|\Upsilon_{n-\kappa}(G)| + \ln\left(\frac{2m_1}{n_1}\right)^{-1}. \tag{21}$$

In particular, if

- *G_1 is s_1-regular, then*

$$\mathcal{E}(G) \geq s_1 + (n-\kappa-1) + \ln|\Upsilon_{n-\kappa}(G)| + \ln s_1^{-1}. \tag{22}$$

- *G is a connected (n,m)-graph with $n \geq 2$ and $\frac{2m}{n} \geq 1$, then*

$$\mathcal{E}(G) \geq \frac{2m}{n} + (n-\kappa-1) + \ln|\Upsilon_{n-\kappa}(G)| + \ln\left(\frac{2m}{n}\right)^{-1}. \tag{23}$$

If $\rho = 1$ then equalities in (21) and (22) hold if and only if $G = \lfloor\frac{n-\kappa}{2}\rfloor K_2 \cup \kappa K_1$. On the contrary, if $\rho > 1$ then equalities in (21) and (22) hold if and only if $G = K_{n-\ell} \cup \kappa K_1 \cup \lfloor\frac{\ell-\kappa}{2}\rfloor K_2$ with $\kappa \leq \ell \leq n-3$, taken $G_1 = K_{n-\ell}$. The inequality in (23) becomes equality if and only if $G = K_n$, see [8].

Proof. Let G_1 be an induced (n_1,m_1)-subgraph of G with $n_1 \geq 1$ and $\rho(G_1) = \rho$. The proof of the inequality follows directly from the proof of Corollary 3 changing the non-negative symmetric matrix R by the adjacency matrix of the graph G and by considering the vector $\mathbf{x}$ such as it was exhibited in Remark 3. At this point recall that, if $\mathbf{x}$ and $\mathbf{y}$, are as in Remark 3 being $\mathbf{y} = \mathbf{e}$, the all ones vector of appropriate order, then $\frac{\mathbf{x}^T A(G)\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \frac{2m_1}{n_1} \leq \rho(G_1) = \rho$, with equality if and only if G_1 is a regular graph (see [6], for example). Recall that the real function $h(x)$ defined in (16) is strictly increasing for $x \geq 1$. From the condition $\frac{2m_1}{n_1} \geq 1$ we have

$$\mathcal{E}(G) \geq h(\rho) = h(\rho(G_1)) \geq h\left(\frac{2m_1}{n_1}\right). \tag{24}$$

Thus, the inequality in (21) follows. If equality holds in (21) then all the inequalities in (24) become equalities and then the nonzero eigenvalue, λ, different from the largest eigenvalue, ρ verifies $|\lambda| = 1$ implying that $\lambda = \pm 1$ and $\rho = \rho(G_1) = \frac{2m_1}{n_1}$ as h is a strict increasing function, thus, G_1 is a regular component with largest eigenvalue equal to ρ. In consequence, if $n_1 = 2$ then $G_1 = K_2$, and G is a union of graphs K_2 and κ isolated vertices. If $n_1 \geq 2$, by the item 1. in Theorem 2 each subset of three vertices of $V(G)$ are the vertices of a complete subgraph of G. In consequence $G_1 = K_{n-\ell}$ with $n-\ell \geq 3$. Since the other non null eigenvalues have absolute values equal to 1, the other components of G must be isolated edges and κ isolated vertices. Thus the graphs in the statement proceed. If G is a connected graph, then considering $G_1 = G$, and from the cases $n_1 = n = 2$ and $n_1 = n \geq 3$ of the above reasoning, we conclude that $G = K_n$. Conversely, one can see that the equalities hold for the graphs in the statement. ∎

From inequalities (21) and (19), we derive the following result.

Corollary 7. *Let G be an (n, m)-graph without isolated vertices, with largest eigenvalue ρ, $\eta(G) = \kappa$ with $0 \leq \kappa \leq n-1$ and let G_1 be an (n_1, m_1) component of G such that $n_1 \geq 2$, $\frac{2m_1}{n_1} \geq 1$ and whose largest eigenvalue is equal to ρ. Therefore*

$$\mathcal{E}(G) \geq \frac{2m_1}{n_1} + (n-\kappa-1) + \ln\left(\frac{2m_1}{n_1}\right)^{-1}. \tag{25}$$

Equality in (25) holds if and only if $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$. In particular, if

- *G_1 is s_1-regular, then*

$$\mathcal{E}(G) \geq s_1 + (n-\kappa-1) + \ln s_1^{-1}. \tag{26}$$

  Equality in (26) holds if and only if $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$.

- *G is a connected (n, m)-graph, then*

$$\mathcal{E}(G) \geq \frac{2m}{n} + (n-\kappa-1) + \ln\left(\frac{2m}{n}\right)^{-1}. \tag{27}$$

  Equality holds, if and only if $G = K_2$.

2.3 Lower bounds for the energy of bipartite graphs with given nullity

In this subsection we deal with bipartite graphs. Recall that if G is bipartite and λ is a nonzero eigenvalue of G, then $-\lambda$ is also an eigenvalue of G, thus, we conclude that the rank of a bipartite graph must be even. In consequence, for the rank r of G we set $r = n - \kappa = 2t$.

Theorem 8. *Let G be a bipartite (n, m)-graph of rank $r = 2t = n - \kappa$, with $t \geq 2$, and largest eigenvalue ρ then*

$$\mathcal{E}(G) \quad \geq \quad 2\rho + (n-\kappa-2) + \ln|\Upsilon_{n-\kappa}(G)| + 2\ln\rho^{-1}. \tag{28}$$

The equality holds in (28) if and only if G has the eigenvalues,

$$\rho, \underbrace{1 \ldots 1}_{t-1 \ times}, \underbrace{0 \ldots, 0}_{\kappa \ times}, \underbrace{-1 \ldots -1}_{t-1 \ times}, -\rho. \tag{29}$$

That is the case, for instance, if $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$, or $H = (K_{t,t} \setminus W) \cup \kappa K_1$, where W is a perfect matching.

Proof. Let G be a bipartite (n,m)-graph of rank $n-\kappa = r = 2t$, $t \geq 2$, then

$$\begin{aligned}
\mathcal{E}(G) &= 2\sum_{j=1}^{t}|\lambda_j| \geq 2\left(\rho + t - 1 + \sum_{j=2}^{t}\ln|\lambda_j|\right)\\
&= 2\left(\rho + t - 1 + \ln\left|\prod_{j=2}^{t}\lambda_j\right|\right)\\
&= 2\left(\rho + t - 1 + \frac{1}{2}\ln\left|\prod_{j=2}^{r}\lambda_j\right|\right)\\
&= 2\left(\rho + t - 1 + \frac{1}{2}\ln|\Upsilon_{n-\kappa}(G)| - \ln\rho\right)\\
&= 2\rho + r - 2 + \ln|\Upsilon_{n-\kappa}(G)| - 2\ln\rho.
\end{aligned}$$

Equality holds if and only if $|\lambda_j| = 1, \quad \forall 2 \leq j \leq t$. By an appropriate labeling of the vertices of $H = (K_{t,t} \setminus W) \cup \kappa K_1$, its adjacency matrix becomes,

$$\begin{pmatrix} 0 & A(K_t) & 0\\ A(K_t) & 0 & 0\\ 0 & 0 & 0\end{pmatrix}$$

and

$$\begin{pmatrix} 0 & A(K_t)\\ A(K_t) & 0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} I_t & I_t\\ I_t & -I_t\end{pmatrix}\begin{pmatrix} A(K_t) & 0\\ 0 & -A(K_t)\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} I_t & I_t\\ I_t & -I_t\end{pmatrix}.$$

Then, considering $\rho = t-1$ the eigenvalues of H are the elements in the list (29). ■

The following result is an immediate consequence of the previous one, the increasing function in (16) and the Rayleigh quotient theory, (see [13]).

Corollary 9. *Let G be a bipartite (n,m)-graph of rank $r = 2t = n-\kappa$, $t \geq 2$ and $\frac{2m}{n} \geq 1$. then*

$$\mathcal{E}(G) \geq \frac{4m}{n} + (n-\kappa-2) + \ln|\Upsilon_{n-\kappa}(G)| + 2\ln\left(\frac{2m}{n}\right)^{-1}. \tag{30}$$

The equality holds in (30) if G has the list of eigenvalues,

$$\frac{2m}{n}, \underbrace{1\ldots 1}_{t-1 \ times}, \underbrace{0\ldots, 0}_{\kappa \ times}, \underbrace{-1\ldots -1}_{t-1 \ times}, -\frac{2m}{n}.$$

That is the case, for instance, if $\kappa = 0$ and $G = K_{t,t} \setminus W$ where W is a perfect matching.

Taking into account Theorem 8 and inequality (19) another lower bound is presented in the next corollary.

Corollary 10. *Let G be a bipartite (n,m)-graph of rank $r = 2t = n - \kappa$, $t \geq 2$ and largest eigenvalue ρ, then*

$$\mathcal{E}(G) \;\geq\; 2\rho + (n - \kappa - 2) + 2\ln\rho^{-1}. \tag{31}$$

The equality holds in (31) if $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$.

The proof of the following corollary is direct and uses the statement in (13).

Corollary 11. *If $n - \kappa = r > 2 + 2\ln\rho$, then the lower bound in (31) improves the lower bound in (8).*

Proof. If the inequality in the statement holds by considering the lower bound in (31) we have

$$\begin{aligned} 2\rho + r - 2 + 2\ln\rho^{-1} &> 2\rho + (2 + 2\ln\rho) - 2 + 2\ln\rho^{-1} \\ &= 2\rho. \end{aligned}$$

Thus, the result follows. ■

Example 1. *Let $t \geq 2$ and consider $(K_{t,t} \setminus W) \cup \kappa K_1$. Therefore, $n = 2t + \kappa$, $r = 2t$, and $\rho = t - 1$. Therefore, the condition in Corollary 11 holds. In fact, the real function $F(x) = x - 1 - \ln(x-1), \quad \forall x > 1$ has a minimum in $x = 2$. Thus $F(x) \geq F(2) = 1$, which implies that $2t - 2 + 2\ln(t-1)^{-1} = 2(t - 1 - \ln(t-1)) \geq 2 > 0$. Thus $r = 2t > 2 + 2\ln(t-1)$ which is the sufficient condition in Corollary 11. Moreover, it is immediate to obtain that $\mathcal{E}(H) = 4t - 4 > 2(t-1) = 2\rho$.*

Using Corollary 9 and Rayleigh quotient the next corollary is obtained.

Corollary 12. *Let G be a bipartite (n,m)-graph of rank $r = 2t$, $t \geq 2$, then*

$$\mathcal{E}(G) \;\geq\; \frac{4m}{n} + (n - \kappa - 2) + 2\ln\left(\frac{2m}{n}\right)^{-1}. \tag{32}$$

3 An increasing sequence of lower bounds for the graph energy

In this section we obtain an increasing sequence of lower bounds for the energy of graphs. In [5], the authors built an increasing sequence, $\{\gamma^{(k)}\}_{k\geq 0}$ of lower bounds for ρ, where,

$$\begin{aligned} \gamma^{(0)} &= \sqrt{\frac{\sum\limits_{i\in V(G)} d^2(i)}{n}}, \\ \gamma^{(1)} &= \sqrt{\frac{\sum\limits_{i\in V(G)} d_2^2(i)}{\sum\limits_{i\in V(G)} d^2(i)}}, \\ &\vdots \\ \gamma^{(k)} &= \sqrt{\frac{\sum\limits_{i\in V(G)} d_{k+1}^2(i)}{\sum\limits_{i\in V(G)} d_k^2(i)}}, \quad \forall k \geq 2. \end{aligned} \tag{33}$$

Then the following results were obtained.

Theorem 13. *[5] Let G be a connected graph with largest eigenvalue ρ. Then*

$$\rho \geq \gamma^{(k+1)} \geq \gamma^{(k)}, \quad \forall k \geq 0,$$

with equality if $A^{k+2}(G)\mathbf{e} = \rho^2 A^k(G)\mathbf{e}, \quad \forall k \geq 0$.

Theorem 14. *[5] Let G be a connected graph, then $\{\gamma^{(k)}\}_{k\geq 0}$ is an increasing sequence and*

$$\lim_{k\to\infty} \gamma^{(k)} = \rho.$$

In this work we achieved to the following results.

Theorem 15. *Let G be an (n,m)-graph with largest eigenvalue ρ and $\eta(G) = \kappa$. Let G_1 be an (n_1, m_1) component with spectral radius ρ and such that $\frac{2m_1}{n_1} \geq 1$. Let $\{\gamma_1^{(k)}\}_{k=0}^{\infty}$ be the increasing sequence defined in (33) for G_1 and h the real continuous function defined in (16). Then $\{h(\gamma_1^{(k)})\}_{k=0}^{\infty}$ is an increasing sequence of lower bounds for $\mathcal{E}(G)$ converging to $h(\rho)$ and*

$$\mathcal{E}(G) \geq h(\rho) \geq h(\gamma_1^{(k+1)}) \geq h(\gamma_1^{(k)}), \quad \forall k \geq 0. \tag{34}$$

If $\rho = 1$ then equality holds for some $k \geq 0$ if and only if $G = \lfloor \frac{n-\kappa}{2} \rfloor K_2 \cup \kappa K_1$. On the contrary, if $\rho > 1$ then equality holds for some $k \geq 0$ if and only if $G = K_{n-\ell} \cup \kappa K_1 \cup \lfloor \frac{\ell-\kappa}{2} \rfloor K_2$, $\kappa \leq \ell \leq n-3$ with $G_1 = K_{n-\ell}$.

Proof. Observe that $\gamma_1^{(k)} \geq 1, \quad \forall k \geq 0$. This is an immediate consequence of Theorem 14 and the fact that

$$\gamma_1^{(0)} = \sqrt{\frac{\sum_{i \in V(G_1)} d_1^2(i)}{n_1}} \geq \sqrt{\frac{2m_1}{n_1}} \geq 1.$$

Since $\{\gamma_1^{(k)}\}_{k=0}^{\infty}$ is an increasing sequence and converges to $\rho(G_1) = \rho$ then, the first statement follows from the continuity and the strict increasing of h. If all inequalities in (34) are equalities, for some k then $\mathcal{E}(G) = h(\rho) = h(\gamma_1^{(k)})$ and we are in the conditions of Theorem 5. Therefore G is as in the statement.

■

Recalling the result in (7) obtained in [8], the result given in [14] is here re-obtained considering $\kappa = 0$.

Corollary 16. *Let G be a non-singular graph of order n. Define the sequence $\{\gamma^{(k)}\}_{k=0}^{\infty}$ as in (33). Then*

$$\mathcal{E}(G) \geq \gamma^{(k)} + (n-1) + \ln |\det A| - \ln \gamma^{(k)}, \tag{35}$$

$\forall k \geq 0$. Equality holds, for some $k \geq 0$, if and only if $G = K_{n-\ell} \cup \lfloor \frac{\ell}{2} \rfloor K_2$, $0 \leq \ell \leq n-2$.

4 Computational experiments

Next some comparatives examples for different values of n are presented.

Using different graphs the lower bounds in the paper are compared. In order to control the differences among the lower bound (6) and the new lower bound in (18) the rank r is given. The energies E, the rank, and the lower bounds in (8), (9), (18), (20), (23) and (27), are compared.

Only the last 4 columns are the lower bounds found in the present work. We begin with $n = 3$:

Adjacency	E	r	(8)	(9)	(18)	(20)	(23)	(27)
K_3	4	3	4	3.4641	4	3.3069	4	3.3069
$K_{1,2}$	2.8284	2	2.8284	2.8284	2.7608	2.0676	2.7388	2.0457

$n = 4:$

Adjacency	E	r	(8)	(9)	(18)	(20)	(23)	(27)
K_4	6	4	6	4.8990	6	4.9014	6	4.9014
$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	5.1231	3	5.1231	4.4721	5.0072	3.6209	4.9700	3.5837
$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	4.9624	4	4.3402	4	4.3953	4.3953	4.3069	4.3069

$n = 5:$

Adjacency	E	r	(8)	(9)	(18)	(20)	(23)	(27)
$\begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{pmatrix}$	6.7299	5	5.2824	4.8990	6.3631	5.6700	6.2177	5.5245
$\begin{pmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$	6.0409	4	5.3711	4.8990	5.3908	4.6977	5.2177	4.5245
C_5	6.4721	5	4	4.4721	6	5.3069	5.3069	5.3069

5 Conclusions

The present work continues the idea of determining lower bounds for the energy of a graph considering the nullity of its adjacency matrix. In this way, it is possible to increase the set of lower bounds for the energy, obtaining together with these lower bounds the (n, m)-graphs with given nullity and minimum energy. When we compare the lower bound in (18) with the lower bound in (28), the arithmetic difference of the second one minus the first one gives $\rho - 1 + \ln \rho^{-1} \geq 0, \quad \forall \rho \geq 1$. The above fact allows us to conclude that the lower bound obtained for bipartite graphs is more efficient.

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