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Some Eigenvalue Properties and New Bounds for the Energy of Extended Adjacency Matrix of Graphs

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Abstract

Let G be a graph with vertex set $V = V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E = E(G)$. In 1994, Yang et al. proposed the extended adjacency matrix, denoted by $A_{ex} = A_{ex}(G)$, which is defined that its (i, j)-entry is equal to $\frac{1}{2}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)$ if the vertices v_i and v_j are adjacent, and 0 otherwise, where d_i is the degree of vertex v_i. In this paper, we first derive some new bounds for the extended spectral radius (η_1) in terms of some significant graph parameters, such as the minimum and maximum degree of G, the chromatic number (χ), the Randić index (R), the modified second Zagreb index (M_2^*), the Symmetric Division Deg index (*SDD*) and so on. Moreover, several eigenvalue properties of extended adjacency matrix are presented. Finally, we characterize some new lower and upper bounds on $\mathcal{E}_{ex}$.

1 Introduction

Eigenvalue-based topological molecular descriptors have played an increasingly important role in chemical research in recent years. Graph energy, introduced by *I.Gutman* [12,13], is a significant and representative eigenvalue-based topological molecular descriptors, since it can be used to approximate the total π-*electron* energy of molecule. Let G be a graph with vertex set $V = V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E = E(G)$. The *adjacent matrix* of the graph G, denoted by $A(G)$, is defined that its (i,j)-entry is equal to 1 if $v_iv_j \in E(G)$ $(v_i \sim v_j)$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \cdots \geq \lambda_n$ be the eigenvalues of $A(G)$. The greatest eigenvalue of λ_1 is usually referred to as the spectral radius of G. The energy of the graph G is defined as

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

Nowadays, relevant researches on graph energy are very popular. Several important conclusions can be found in the recent papers [5,6,14,16,21], and the references cited therein.

In 1994, Yang et al. [26] proposed the extended adjacency matrix of the graph G, which is denoted by $A_{ex} = A_{ex}(G)$. An element of this matrix can be defined in the following equations:

$$a_{ij}^{ex} = \begin{cases} \frac{1}{2}(\frac{d_i}{d_j} + \frac{d_j}{d_i}), & \text{if vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

which d_i and d_j are the degrees of the vertices v_i and v_j, respectively.

Similarly, let $\eta_1 \geq \eta_2 \cdots \geq \eta_n$ be eigenvalues of $A_{ex}(G)$. The greatest eigenvalue of η_1 is usually viewed as the extended spectral radius of G. The extended graph energy of the graph G is defined as

$$\mathcal{E}_{ex} = \mathcal{E}_{ex}(G) = \sum_{i=1}^{n} |\eta_i|,$$

(see [26]).

Some papers [2, 7, 15, 17, 25] on extended graph energy published in past three years have established some mathematical properties of $\mathcal{E}_{ex}$ and contributed to further research on this matter.

In the later part of this paper we shall need some important classical graph parameters. The maximum and minimum degrees of the graph G are denoted by Δ and δ, respectively. The *chromatic number* of G is the smallest number of colours needed to colour a graph G, denoted by $\chi(G)$. The *Randić index* of G, denoted by $R(G)$, is defined as

$$R = R(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_id_j}}.$$

The *modified second Zagreb index* of G [22], is defined as

$$M_2^* = M_2^*(G) = \sum_{v_iv_j \in E(G)} \frac{1}{d_id_j},$$

for lower and upper bounds on M_2^*, see [19]. The *Symmetric Division Deg index* [24] is

$$SDD = SDD(G) = \sum_{v_iv_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right),$$

and relevant researches on *SDD*-index can refer to [1,9,20,23].

In this paper, we first derive some new bounds for the extended spectral radius (η_1) in terms of some significant graph parameters, such as the minimum and maximum degree of G, the chromatic number (χ), the Randić index (R), the modified second Zagreb index (M_2^*), the Symmetric Division Deg index (*SDD*) and so on. Moreover, several eigenvalue properties of extended adjacency matrix are presented. Finally, we characterize some new lower and upper bounds on $\mathcal{E}_{ex}$.

2 Lemmas

In this section, we list some previously known results which are necessary for subsequent part.

Lemma 1. *(Rayleigh-Ritz [27]) If B is symmetric $n \times n$ matrix with eigenvalues $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$, then for any $\boldsymbol{x} \in R^n$, such that $\boldsymbol{x} \neq 0$,*

$$\boldsymbol{x}^T B \boldsymbol{x} \leq \rho_1 \boldsymbol{x}^T \boldsymbol{x}.$$

Equality holds if and only if $\boldsymbol{x}$ is an eigenvalue of B corresponding to the largest eigenvalue ρ_1.

Lemma 2. *[18] Let $B = (b_{ij})$ and $C = (c_{ij})$ be symmetric, non-negative matrices of order n. If $B \geq C$, i.e. $b_{ij} \geq c_{ij}$ for all i, j, then $\rho_1(B) \geq \rho_1(C)$, where ρ_1 is the largest eigenvalue.*

Lemma 3. *[3] The spectrum of an empty graph of order n is $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 0$, the spectrum of a complete graph K_n is $\lambda_1 = n-1$, $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$, the spectrum of a complete bipartite graph $K_{p,q}$ with $p + q = n$ is $\lambda_1 = \sqrt{pq}$, $\lambda_2 = \cdots \lambda_{n-1} = 0$, $\lambda_n = -\sqrt{pq}$, and that of a regular graph G of degree k is $k = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.*

Lemma 4. *[4] Let G be a graph of order n with m edges and minimum (resp. maximum) degree $\delta \geq 1$ (resp.Δ). Then*

$$\lambda_1 \leq \sqrt{2m - \delta(n-1) + (\delta - 1)\Delta},$$

with equality holding if and only if G is regular, a star plus copies of K_2, or a complete graph plus a regular graph with smaller degree of vertices.

Lemma 5. *[8] For any connected graph, $\lambda_1 \leq \sqrt{2m(\chi - 1)/\chi}$.*

Lemma 6. *[7] Let G be a graph of order n with maximum degree Δ and minimum degree δ. Then*

$$\eta_1 \leq \left[1 + \frac{(\Delta - \delta)^2}{2\delta^2}\right] \lambda_1,$$

with equality holding if and only if G is regular.

Lemma 7. *[7] Let G be a graph of order n. Then $|\eta_1| = |\eta_2| = \cdots = |\eta_n|$ if and only if $G \cong \overline{K}_n$ or $G \cong \frac{n}{2}K_2$.*

3 Eigenvalue properties of extended adjacency matrix of graphs

We state here some equations which show the elementary properties of extended adjacency matrix of G.

$$\sum_{i=1}^{n} \eta_i = \sum_{i=1}^{n} \lambda_i = 0, \ \sum_{i=1}^{n} \lambda_i^2 = 2\sum_{i<j}(a_{ij})^2 = 2m, \tag{1}$$

$$\sum_{i=1}^{n} \eta_i^2 = 2\sum_{i<j}(a_{ij}^{ex})^2 = \frac{1}{2}\sum_{v_iv_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)^2. \tag{2}$$

The following two theorems present some new bounds for the extended spectral radius η_1.

Theorem 8. *Let G be a non-empty graph of order n with m edges, maximum degree Δ and minimum degree δ. Then*

(i)

$$\eta_1 \leq \frac{1}{2}\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right)\sqrt{2m(\chi - 1)/\chi},$$

with equality holding if and only if G is the direct sum of r complete $(\frac{n}{n-rk})$-part graph $K_{\frac{n-rk}{r}, \frac{n-rk}{r}, \cdots, \frac{n-rk}{r}}$ or G is the direct sum of r complete bipartite graph $K_{p,q}$, with $p + q = \frac{n}{r}$.

(ii)

$$\eta_1 \leq \left[1 + \frac{(\Delta - \delta)^2}{2\delta^2}\right]\sqrt{2m(\chi - 1)/\chi},$$

with equality holding if and only if G is the direct sum of r complete $(\frac{n}{n-rk})$-part graph $K_{\frac{n-rk}{r}, \frac{n-rk}{r}, \cdots, \frac{n-rk}{r}}$.

(iii)

$$\eta_1 \leq \left[1 + \frac{(\Delta - \delta)^2}{2\delta^2}\right]\sqrt{2m - \delta(n - 1) + (\delta - 1)\Delta},$$

with equality holding if and only if G is a regular.

Proof. (i) For any edge $v_iv_j \in E(G)$, we have

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} \leq \frac{\Delta}{\delta} + \frac{\delta}{\Delta} \tag{3}$$

with equality holding if and only if $d_i = \Delta$, $d_j = \delta$ or $d_i = \delta$, $d_j = \Delta$.

Consider the following two cases.

Case 1. If $d_i = d_j = \Delta = \delta$, it is obvious that G is a regular graph. In this case, $A_{ex}(G) = A(G)$.

Case 2. If $\Delta \neq \delta$, then we let $p = \Delta$, $q = \delta$ or $p = \delta$, $q = \Delta$. It is easy to obtain that G is the direct sum of r complete bipartite graph $K_{p,q}$, with $p + q = \frac{n}{r}$.

If ρ_1 is the largest eigenvalue of the matrix $\frac{1}{2}(\frac{\Delta}{\delta} + \frac{\delta}{\Delta})A(G)$, then by Lemma 2, we know that $\eta_1 \leq \rho_1$. In view of (3), then

$$\eta_1 \leq \frac{1}{2}\left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right)\lambda_1, \tag{4}$$

with equality holding if and only if G is a regular graph or G is the direct sum of r complete bipartite graph $K_{p,q}$ $(p + q = \frac{n}{r})$.

For a connected regular graph G of degree k, $m = \dfrac{nk}{2}$. Let $\lambda_1 = \sqrt{2m(\chi - 1)/\chi}$, by Lemma 3, then

$$k = \sqrt{nk(\chi(G) - 1)/\chi(G)}.$$

Thus,

$$\frac{\chi(G) - 1}{\chi(G)} = \frac{k}{n},$$

where $k = 1, 2, \cdots, n-1$. Since $\chi(G)$, k and n are integer, then the following equation system is easy to obtained:

$$\begin{cases} k = 1, \ \chi(G) = \frac{n}{n-1}, \\ k = 2, \ \chi(G) = \frac{n}{n-2}, \\ \qquad \vdots \\ k = n-3, \ \chi(G) = \frac{n}{3}, \\ k = n-2, \ \chi(G) = \frac{n}{2}, \\ k = n-1, \ \chi(G) = n. \end{cases}$$

By derivation, we can know that for a connected regular graph G of degree k, $\lambda_1 = \sqrt{2m(\chi - 1)/\chi}$ if and only if G is the complete $(\frac{n}{n-k})$-part graph $K_{n-k,n-k,\cdots,n-k}$. If $\lambda_1 = \lambda_2 = \cdots = \lambda_r = k$, by the Perron-Frobenius theorem, one can see that the graph G is the direct sum of r complete $(\frac{n}{n-rk})$-part graph $K_{\frac{n-rk}{r},\frac{n-rk}{r},\cdots,\frac{n-rk}{r}}$.

In Case 2, $\chi(K_{p,q}) = 2$, and $m(K_{p,q}) = pq$. If $p+q = n$, then we have $\sqrt{2m(\chi - 1)/\chi} = \sqrt{m} = \sqrt{pq} = \lambda_1(K_{p,q})$. Thus, $G \cong K_{p,q}$. Similarly, if $\lambda_1 = \lambda_2 = \cdots = \lambda_r$, one can check that G is the direct sum of r complete bipartite graph $K_{p,q}$, with $p + q = \frac{n}{r}$.

On the whole, from Lemma 3, Lemma 5 and (4), we can get

$$\eta_1 \leq \frac{1}{2}\left(\frac{\delta}{\Delta}+\frac{\Delta}{\delta}\right)\sqrt{2m(\chi-1)/\chi}$$

with equality holding if and only if G is the direct sum of r complete $(\frac{n}{n-rk})$-part graph $K_{\frac{n-rk}{r},\frac{n-rk}{r},\cdots,\frac{n-rk}{r}}$ or G is the direct sum of r complete bipartite graph $K_{p,q}$, with $p+q=\frac{n}{r}$.

(ii)-(iii) In view of Lemma 4 - 6 and the proofs of Theorem 8 (i), it is easy to obtain the results of Theorem 8 (ii)-(iii).

This completes the proofs of Theorem 8. ■

Theorem 9. *Let G be a non-empty graph of order n with m edges and minimum degree δ. Then*

(i)

$$\eta_1 \geq \frac{4\delta^2 M_2^*}{n} - \frac{2m}{n} \geq \frac{4\delta^2 R^2}{nm} - \frac{2m}{n}, \tag{5}$$

with all equalities holding if and only if G is a regular graph.

(ii)

$$\eta_1 \geq \frac{SDD}{n}, \tag{6}$$

with equality holding if and only if G is a regular graph.

(iii)

$$\eta_1 \geq \frac{2m}{n}, \tag{7}$$

with equality holding if and only if G is a regular graph.

Proof. (i) Let $\mathbf{x}=(x_1,x_2,\cdots,x_n)^T$ be any unit vector in R^n. Then we have

$$\begin{aligned}\mathbf{x}^T A_{ex}(G)\mathbf{x} &= \sum_{v_iv_j\in E(G)}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)x_ix_j \\ &= \sum_{v_iv_j\in E(G)}\frac{(d_i+d_j)^2}{d_id_j}x_ix_j - 2\sum_{v_iv_j\in E(G)}x_ix_j \\ &\geq 4\delta^2\sum_{v_iv_j\in E(G)}\frac{1}{d_id_j}x_ix_j - 2\sum_{v_iv_j\in E(G)}x_ix_j. \end{aligned}\tag{8}$$

Suppose $\mathbf{x}=(\frac{1}{\sqrt{n}},\frac{1}{\sqrt{n}},\cdots,\frac{1}{\sqrt{n}})$, then

$$\mathbf{x}^T A_{ex}(G)\mathbf{x} \geq \frac{4\delta^2 M_2^*}{n} - \frac{2m}{n}. \tag{9}$$

By the Cauchy-Schwarz inequality,

$$\left(\sum_{v_iv_j\in E(G)}\frac{1}{\sqrt{d_id_j}}\right)^2 \leq m\sum_{v_iv_j\in E(G)}\frac{1}{d_id_j}.$$

Thus, we can get $M_2^* \geq \frac{R^2}{m}$. Equality holds if and only if G is a regular graph or G is the direct sum of r complete bipartite graph $K_{p,q}$, with $p+q=\frac{n}{r}$. Combining with (9), we have

$$\mathbf{x}^T A_{ex}(G)\mathbf{x} \geq \frac{4\delta^2 M_2^*}{n} - \frac{2m}{n} \geq \frac{4\delta^2 R^2}{nm} - \frac{2m}{n}.$$

By Lemma 1, we get

$$\eta_1 \geq \mathbf{x}^T A_{ex}(G)\mathbf{x} \geq \frac{4\delta^2 M_2^*}{n} - \frac{2m}{n} \geq \frac{4\delta^2 R^2}{nm} - \frac{2m}{n}.$$

Assume now that all equalities hold in (5), then all the above inequalities must be equalities. If equality holds in (8), then $d_1 = d_2 = \cdots = d_n = \delta$. Further, from $\eta_1 = \mathbf{x}^T A_{ex}(G)\mathbf{x}$, it follows that $\mathbf{x} = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \cdots, \frac{1}{\sqrt{n}})^T$ is an eigenvector corresponding to the eigenvalue η_1. Hence G is a regular graph.

This completes the proofs of Theorem 9 (i).

(ii) Similarly, let $\mathbf{x} = (x_1, x_2, \cdots, x_n)^T$ be any unit vector in R^n. Then

$$\mathbf{x}^T A_{ex}(G)\mathbf{x} = \sum_{v_iv_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) x_i x_j. \tag{10}$$

Putting $\mathbf{x} = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \cdots, \frac{1}{\sqrt{n}})$ into (10), we have

$$\mathbf{x}^T A_{ex}(G)\mathbf{x} = \frac{1}{n} \sum_{v_iv_j \in E(G)} (\frac{d_i}{d_j} + \frac{d_j}{d_i}) = \frac{SDD}{n}.$$

Then by Lemma 1, $\eta_1 \geq \mathbf{x}^T A_{ex}(G)\mathbf{x} = \frac{SDD}{n}$. Equality holds if and only if $\mathbf{x} = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \cdots, \frac{1}{\sqrt{n}})$ is an eigenvector corresponding to the eigenvalue η_1.

Since the extended spectrum of a regular graph coincides with the ordinary graph spectrum, one can easily check that G is a regular graph.

This completes the proofs of 9 (ii).

(iii) Let $\mathbf{x} = (x_1, x_2, \cdots, x_n)^T$ be any unit vector in R^n. Based on fundamental inequality, we have

$$\mathbf{x}^T A_{ex}(G)\mathbf{x} = \sum_{v_iv_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) x_i x_j \geq 2 \sum_{v_iv_j \in E(G)} x_i x_j. \tag{11}$$

with equality holding if and only if $d_i = d_j$ for any $v_iv_j \in E(G)$.

Putting $\mathbf{x} = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \cdots, \frac{1}{\sqrt{n}})$ into (11),then,

$$\eta_1 \geq \mathbf{x}^T A_{ex}(G)\mathbf{x} \geq \frac{2m}{n}. \tag{12}$$

Based on the proofs of Theorem 9 (i)-(ii), similarly, we can prove that all equalities hold in (12) if and only if G is a regular graph.

This completes the proofs of Theorem 9 (iii). ■

Then we give two theorems which show some eigenvalue properties of extended adjacency matrix of several special graphs.

Theorem 10. *For a bipartite graph of order n, then $\eta_1 = -\eta_n$. The extended spectrum of a complete bipartite graph $K_{p,q}$ is $\eta_1 = \frac{1}{2}\left(\frac{p}{q}+\frac{q}{p}\right)\sqrt{pq}$, $\eta_2 = \cdots = \eta_{n-1} = 0$, $\eta_n = -\frac{1}{2}\left(\frac{p}{q}+\frac{q}{p}\right)\sqrt{pq}$, and that of a complete graph K_n is $\eta_1 = n-1$, $\eta_2 = \eta_3 = \cdots = \eta_n = -1$.*

Proof. The extended adjacency matrix of a bipartite graph has the form

$$A_{ex} = \begin{pmatrix} 0 & C \\ C^T & 0 \end{pmatrix}.$$

The extended spectrum of a bipartite graph is symmetric. If $(\mathbf{u}, \mathbf{v})^T$ is an eigenvector with eigenvalue ρ, then $(\mathbf{u}, -\mathbf{v})^T$ is an eigenvector with eigenvalue $-\rho$. Since η_1 is the extended spectral radius of bipartite graph G, then we have $\eta_1 = -\eta_n$.

It is obvious that for a complete bipartite graph $K_{p,q}$, $A_{ex}(K_{p,q}) = \frac{1}{2}(\frac{p}{q}+\frac{q}{p})A(K_{p,q})$, and for a complete graph K_n, $A_{ex}(K_n) = A(K_n)$. By Lemma 3, one can easily obtain the conclusions. ■

Theorem 11. *The extended adjacency matrix of graphs has only one distinct eigenvalue if and only if G is an empty graph; has two distinct eigenvalues $\mu_1 > \mu_2$ multiplicities m_1 and m_2 if and only if G is the direct sum of m_1 complete graphs of order $\mu_1 + 1$. In this case, $\mu_2 = -1$ and $m_2 = m_1\mu_1$.*

Proof. Since $A_{ex}(G)$ is a real symmetric matrix, if $A_{ex}(G)$ has one eigenvalue μ, then the minimal polynomial $m(x) = x - \mu$. Thus $A_{ex} = \mu I$. Since A_{ex} is zero on the diagonal, $\mu = 0$ and $A_{ex} = 0$. Thus G is an empty graph,

If G has two distinct eigenvalues $\mu_1 > \mu_2$, with multiplicities m_1 and m_2, respectively. Since

$$\sum_{i=1}^{n} \eta_i = 0,$$

Then we have the following equations:

$$m_1 + m_2 = n, \;\; m_1\mu_1 + m_2\mu_2 = 0. \tag{13}$$

By the Perron-Frobenius theorem, for any connected graph Γ, the largest eigenvalue of $A_{ex}(\Gamma)$ $(\rho_1(\Gamma))$ has multiplicity 1. If $\rho_1(\Gamma)$ has multiplicity r, then graph Γ has r connected branches.

Let $l = \dfrac{m_2}{m_1}$, and we assert that l is a positive integer. In fact, by adjusting the label of the vertex of graph G, we have

$$A_{ex} = \begin{bmatrix} Q_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & Q_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & Q_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & Q_{m_1-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & Q_{m_1} \end{bmatrix}_{n\times n} \tag{14}$$

where $Q_i = A_{ex}(H_i)$ $(i = 1, 2, \cdots, m_1)$ has distinct eigenvalues $\mu_1 > \mu_2$ with multiplicities 1 and t_i. In this case, $\sum_{i=1}^{m_1} t_i = m_2$. For any connected branches H_i, $\mu_1 + t_i\mu_2 = 0$. One can easily check that $t_1 = t_2 = \cdots = t_{m_1} = l$.

Therefore, $l = \dfrac{m_2}{m_1}$ is a positive integer, then

$$m_1(l + 1) = n, \ \mu_1 = -l\mu_2.$$

Now $Q_i = |\mu_2| A_{ex}(K_{\frac{\mu_1}{|\mu_2|}+1}) = |\mu_2| A(K_{\frac{\mu_1}{|\mu_2|}+1})$, with $i = 1, 2, \cdots, m_1$. From Lemma 3, we get $\mu_2 = -1$ and $\mu_1 = \lambda_1 = l$. It is obvious that G is the direct sum of m_1 complete graphs of order $\mu_1 + 1$. In this case, $\mu_2 = -1$ and $m_2 = m_1\mu_1$.

■

4 Bounds for the energy of extended adjacency matrix of graphs

The following theorems show some new upper and lower bounds of extended energy of graphs.

Theorem 12. *Let G be a non-empty graph of order n and with m edges, maximum degree Δ and minimum degree δ. Then*

(i)
$$\mathcal{E}_{ex}(G) \le \frac{n}{2}\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right)\sqrt{2m(\chi - 1)/\chi},$$
with equality holding if and only if $G \cong \frac{n}{2}K_2$.

(ii)
$$\mathcal{E}_{ex}(G) \le n\left[1 + \frac{(\Delta - \delta)^2}{2\delta^2}\right]\sqrt{2m(\chi - 1)/\chi},$$
with equality holding if and only if $G \cong \frac{n}{2}K_2$.

(iii)
$$\mathcal{E}_{ex}(G) \le n\left[1 + \frac{(\Delta - \delta)^2}{2\delta^2}\right]\sqrt{2m - \delta(n - 1) + (\delta - 1)\Delta},$$
with equality holding if and only $G \cong \frac{n}{2}K_2$.

Proof. Since
$$\mathcal{E}_{ex}(G) = \sum_{i=1}^{n} |\eta_i| \le n|\eta_1|,$$
with equality holding if and only if $|\eta_1| = |\eta_2| = \cdots = |\eta_n|$.

From Lemma 7 and Theorem 8, it is easy to obtain the conclusions. ■

Theorem 13. *Let G be a non-empty graph of order n with m edges, minimum degree δ. Then*

(i)
$$\mathcal{E}_{ex}(G) \geq \frac{8\delta^2}{n} M_2^* - \frac{4m}{n} \geq \frac{8\delta^2}{nm} R^2 - \frac{4m}{n}.$$
This lower bounds achieved for $G \cong K_n$ *or* $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

(ii)
$$\mathcal{E}_{ex}(G) \geq \frac{2}{n} SDD.$$
This lower bounds achieved for $G \cong K_n$ *or* $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

(iii)
$$\mathcal{E}_{ex}(G) \geq \frac{4m}{n}.$$
This lower bounds achieved for $G \cong K_n$ *or* $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Proof. Since
$$\mathcal{E}_{ex}(G) = \sum_{i=1}^{n} |\eta_i| = 2 \sum_{i=1, \eta_i \geq 0}^{n} |\eta_i| \geq 2|\eta_1|. \tag{15}$$

Equality holds in (15) if and only if $\sum_{i=2}^{n} |\eta_i| = \eta_1$. Combining with Theorem 9 and Theorem 10, one can check that all equalities will hold if $G \cong K_n$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$. ■

Considering the case of extended energy, Gutman [15] defined a parameter M as $M = \sum_{i<j} (a_{ij}^{ex})^2$. Then we have $\sum_{i=1}^{n} \eta_i^2 = 2M$. Koolen and Moulton provided a new method to obtain upper bounds of graph energy and discussed the maximal energy graphs (see [10]) and the maximal energy bipartite graphs (see [11]) in their papers published in 2001 and 2003, respectively. Inspired by Gutman [15], Koolen and Moulton [10, 11], we will derive the Koolen-Moulton bounds of extended energy of graphs and bipartite graphs in the following two theorems.

By the Cauchy-Schwarz inequality, then
$$(\sum_{i=2}^{n} |\eta_i|)^2 \leq (n-1) \sum_{i=2}^{n} |\eta_i|^2, \tag{16}$$
with equality holding if and only if $|\eta_2| = |\eta_3| = \cdots = |\eta_n|$.

Theorem 14. *Let* G *be a non-empty graph of order* n *with* m *edges. Then*

(i)
$$\mathcal{E}_{ex}(G) \leq \tau + \sqrt{(n-1)[2M - \tau^2]},$$
where $\tau = max\left\{\sqrt{\frac{2M}{n}}, \frac{4\delta^2 M_2^* - 2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$. *Equality holds if and only if* $G \cong K_n$ *or* $G \cong \frac{n}{2} K_2$.

(ii)
$$\mathcal{E}_{ex}(G) \leq \tau + \sqrt{(n-1)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}) SDD - \tau^2\right]},$$

where $\tau = max\left\{\sqrt{\frac{(\delta^2+\Delta^2)SDD}{2n\Delta\delta}}, \frac{4\delta^2 M_2^*-2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$. *Equality holds if and only if* $G \cong K_n$ *or* $G \cong \frac{n}{2}K_2$.

Proof. By (2), (3), (16) and (17), we have

(i)

$$\mathcal{E}_{ex}(G) \le |\eta_1| + \sqrt{(n-1)\sum_{i=2}^{n}|\eta_i|^2} \tag{17}$$
$$= |\eta_1| + \sqrt{(n-1)[2M - |\eta_1|^2]}$$

with equality holding in (17) if and only if $|\eta_2| = |\eta_3| = \cdots = |\eta_n|$.

(ii)

$$\mathcal{E}_{ex}(G) \le |\eta_1| + \sqrt{(n-1)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})\sum_{v_iv_j \in E(G)}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) - |\eta_1|^2\right]} \tag{18}$$
$$= |\eta_1| + \sqrt{(n-1)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})SDD - |\eta_1|^2\right]}$$

with equality holding in (18) if and only if $|\eta_2| = |\eta_3| = \cdots = |\eta_n|$, and $d_i = \Delta$, $d_j = \delta$ or $d_i = \delta$, $d_j = \Delta$.

Since the function $g_1(z) = z + \sqrt{(n-1)[2M - z^2]}$ decreases for $\sqrt{\frac{2M}{n}} \le z \le \sqrt{2M}$, and the function $h_1(z) = z + \sqrt{(n-1)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})SDD - z^2\right]}$ decreases for $\sqrt{\frac{(\delta^2+\Delta^2)SDD}{2n\Delta\delta}} \le z \le \sqrt{(\frac{\Delta}{\delta} + \frac{\delta}{\Delta})SDD}$. By Theorem 2,

(i)

$$\mathcal{E}_{ex}(G) \le \tau + \sqrt{(n-1)[2M - \tau^2]}, \tag{19}$$

where $\tau = \max\left\{\sqrt{\frac{2M}{n}}, \frac{4\delta^2 M_2^*-2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$.

(ii)

$$\mathcal{E}_{ex}(G) \le \tau + \sqrt{(n-1)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})SDD - \tau^2\right]}, \tag{20}$$

where $\tau = \max\left\{\sqrt{\frac{(\delta^2+\Delta^2)SDD}{2n\Delta\delta}}, \frac{4\delta^2 M_2^*-2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$.

Then we consider the following two cases.

Case 1. If $\eta_1 = |\eta_2| = \cdots = |\eta_n|$, by Lemma 7, then $G \cong \frac{n}{2}K_2$. For $\frac{n}{2}K_2$, $\frac{4\delta^2 M_2^*-2m}{n} = \frac{SDD}{n} = \frac{2m}{n} = \sqrt{\frac{2M}{n}}$, and $\Delta = \delta = 1$.

Case 2. If $\eta_1 > |\eta_2| = \cdots = |\eta_n|$, by Theorem 11, then $G \cong K_n$. For K_n, $\frac{4\delta^2 M_2^*-2m}{n} = \frac{SDD}{n} = \frac{2m}{n} \ge \sqrt{\frac{2M}{n}}$, and $\Delta = \delta = n-1$.

In summary, equality holds in (19) and (20) if and only if $G \cong K_n$ or $G \cong \frac{n}{2}K_2$. ■

Theorem 15. *Let G be a bipartite graph of order n with m edges. Then*

(i)

$$\mathcal{E}_{ex}(G) \le 2\tau + \sqrt{(n-2)[2M - 2\tau^2]},$$

where $\tau = max\left\{\sqrt{\frac{2M}{n}}, \frac{4\delta^2 M_2^* - 2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$. *This upper bound is achieved for* $G \cong K_{\frac{n}{2},\frac{n}{2}}$, *or* $G \cong \frac{n}{2}K_2$.

(ii)

$$\mathcal{E}_{ex}(G) \le 2\tau + \sqrt{(n-2)[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})SDD - 2\tau^2]},$$

where $\tau = max\left\{\sqrt{\frac{(\delta^2+\Delta^2)SDD}{2n\Delta\delta}}, \frac{4\delta^2 M_2^* - 2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$. *This upper bound is achieved for* $G \cong K_{\frac{n}{2},\frac{n}{2}}$, *or* $G \cong \frac{n}{2}K_2$.

Proof. Since G is a bipartite graph, we have $\eta_1 = -\eta_n$. By the Cauchy-Schwarz inequality,

$$\sum_{i=2}^{n-1} |\eta_i| \le \sqrt{(n-2)\sum_{i=2}^{n-1} |\eta_i|^2} \tag{21}$$

Hence,

(i)

$$\begin{aligned}\mathcal{E}_{ex}(G) &\le 2|\eta_1| + \sqrt{(n-2)\sum_{i=2}^{n-1}|\eta_i|^2} \\ &= 2|\eta_1| + \sqrt{(n-2)\left[2M - 2|\eta_1|^2\right]}\end{aligned}$$

with equality holding if and only if $|\eta_2| = |\eta_3| = \cdots = |\eta_{n-1}|$.

(ii)

$$\begin{aligned}\mathcal{E}_{ex}(G) &\le 2|\eta_1| + \sqrt{(n-2)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})\sum_{v_iv_j \in E(G)}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) - 2|\eta_1|^2\right]} \\ &= 2|\eta_1| + \sqrt{(n-2)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})SDD - 2|\eta_1|^2\right]}\end{aligned}$$

with equality holding if and only if $|\eta_2| = |\eta_3| = \cdots = |\eta_{n-1}|$, and $d_i = \Delta$, $d_j = \delta$ or $d_i = \delta$, $d_j = \Delta$.

Note that the function $g_2(z) = 2z + \sqrt{(n-2)\left[2M - 2z^2\right]}$ decreases for $\sqrt{\frac{2M}{n}} \le z \le \sqrt{2M}$, and the function $h_2(z) = 2z + \sqrt{(n-2)\left[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})SDD - 2z^2\right]}$ decreases for $\sqrt{\frac{(\delta^2+\Delta^2)SDD}{2n\Delta\delta}} \le z \le \sqrt{(\frac{\Delta}{\delta} + \frac{\delta}{\Delta})SDD}$. Based on Theorem 2, we have

(i)

$$\mathcal{E}_{ex}(G) \leq 2\tau + \sqrt{(n-2)[2M - 2\tau^2]}, \tag{22}$$

where $\tau = \max\left\{\sqrt{\frac{2M}{n}}, \frac{4\delta^2 M_2^* - 2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$.

(ii)

$$\mathcal{E}_{ex}(G) \leq 2\tau + \sqrt{(n-2)[\frac{1}{2}(\frac{\delta}{\Delta} + \frac{\Delta}{\delta})SDD - 2\tau^2]}, \tag{23}$$

where $\tau = \max\left\{\sqrt{\frac{(\delta^2+\Delta^2)SDD}{2n\Delta\delta}}, \frac{4\delta^2 M_2^* - 2m}{n}, \frac{SDD}{n}, \frac{2m}{n}\right\}$.

By Lemma 7 and Theorem 11, one can check that equality will hold in (22) and (23) if $G \cong K_{\frac{n}{2},\frac{n}{2}}$ or $G \cong \frac{n}{2}K_2$. ■

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