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Bounds on Nirmala energy of graphs

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Abstract. The Nirmala matrix of a graph and its energy have recently defined. In this paper, we establish some features of the Nirmala eigenvalues. Then we propose various bounds on the Nirmala spectral radius and energy. Moreover, we derive a bound on the Nirmala energy including graph energy and maximum vertex degree.

1 Introduction and Preliminaries

Topological indices that allow to approach molecular structures with regards to mathematics and chemistry, are graph invariants that predict properties such as boiling point, viscosity, radius. The first of these is the Wiener index [22], is used to establish correlations with some physicochemical and thermodynamic parameters of chemical compounds. For other topological indices see also [6, 12, 17].

Let G be a simple graph composed of a vertex set V and edge set E with cardinality n and e, respectively. $u, v \in V$ are adjacent if there is an edge linking them and denoted by $u \sim v$ or $uv \in E$. The neighbourhood N_u of a vertex u is $N_u = \{x \in V : x \sim u\}$. The degree of u, d_u, is the cardinality of N_u. Let Δ, δ be the maximum and minimum vertex degrees. Throughout this work, K_n and $K_{p,q}$ $(p + q = n)$ stand for the complete graph and complete

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bipartite graph with n vertices. $\overline{G}$ stands for the complement of G. The first Zagreb and Nirmala index of G are introduced as

$$Zg(G) = \sum_{u \in V} d_u^2 = \sum_{u \sim v} (d_u + d_v)$$
$$N(G) = \sum_{u \sim v} \sqrt{d_u + d_v}$$

in [12, 17]. Further studies about these indices can be followed from [9, 18].

Let ϑ_i be the eigenvalues of the adjacency matrix A with $\vartheta_1 \geq \vartheta_2 \geq \ldots \geq \vartheta_n$. The energy of G is given in [13] as $En(G) = \sum_{i=1}^{n} |\vartheta_i|$. This definition takes its motivation from Hückel molecular orbital total π-electron energy. Inspired by this study, many graph energy variants are defined and extensive studies are carried out on energy bounds (see [4],[16],[23]). Various applications of graph energy can be found in network analysis [21], computer science [3] and process analysis [10].

The Nirmala matrix $A_N = A_N(G) = (n_{ij})$ of G is an order n matrix, where

$$n_{ij} = \begin{cases} \sqrt{d_i + d_j} & i \sim j \\ 0 & otherwise \end{cases},$$

defined in [11]. The eigenvalues of A_N are named as Nirmala eigenvalues of G with $\nu_1 \geq \nu_2 \geq \ldots \geq \nu_n$, where ν_1 is often called as Nirmala spectral radius. For brevity, we will use N-eigenvalue instead of Nirmala eigenvalue. The Nirmala energy of G is presented [11] as

$$En_N(G) = \sum_{i=1}^{n} |\nu_i|.$$

In this work, firstly some features of the N-eigenvalues are examined. Then novel bounds on ν_1 and $En_N(G)$ including the graph invariants Δ, δ, e, Zg are obtained.

Now, we may present some primaries.

Lemma 1 ([15]) *Let* $B, C \in \mathbb{C}^{n \times n}$ *be nonnegative symmetric matrices with greatest eigenvalue* ϑ_1. *If* $B \geq C$, *then* $\vartheta_1(B) \geq \vartheta_1(C)$.

Lemma 2 ([11]) *Let* ν_1 *be the greatest N-eigenvalue, then*

$$\nu_1 \geq \frac{2N(G)}{n},$$

with equality iff G *is regular.*

2 Bounds for Nirmala eigenvalues and energy

Firstly, some features of the N-eigenvalues will be given.

Lemma 3 *Let* G *be a graph. Then*

(i) $tr(A_N) = 0$,

(ii) $tr(A_N^2) = 2Zg$,

(iii) $tr(A_N^3) = 2\sum_{i\sim j}\sqrt{d_i + d_j} + \sum_{i\sim k,\ k\sim j}\sqrt{d_i + d_k}\sqrt{d_k + d_j}$,

where $tr\,(.)$ *denotes trace of a matrix.*

Proof. (i) and (ii) can be followed by [11]. Clearly, $\left(A_N^2\right)_{ii} = \sum_{i\sim j}(d_i + d_j)$. Let $k \in V$, for $i \neq j$ we get $(A_N^2)_{ij} = \sum_{i\sim k,k\sim j}\sqrt{d_i + d_k}\sqrt{d_k + d_j}$. Then

$$\left(A_N^3\right)_{ii} = \sum_{j=1}^{n} n_{ij}\left(A_N^2\right)_{ji} = \sum_{i\sim j}\sqrt{d_i + d_j}\sum_{i\sim k,\ k\sim j}\sqrt{d_i + d_k}\sqrt{d_k + d_j},$$

$$\begin{aligned} tr(A_N^3) =& \sum_{i\in V}\left(\sum_{i\sim j}\sqrt{d_i + d_j}\sum_{i\sim k,\ k\sim j}\sqrt{d_i + d_k}\sqrt{d_k + d_j}\right) \\ =& 2\sum_{i\sim j}\sqrt{d_i + d_j}\sum_{i\sim k,\ k\sim j}\sqrt{d_i + d_k}\sqrt{d_k + d_j}. \end{aligned}$$

□

Lemma 4 *Let* G *be a graph of order* $n\,(\geq 2)$*. Then the assertions hold as follows.*

(i) If G *is bipartite, then* $\nu_i = -\nu_{n-i+1}$, $i = 1, 2, ..., \left\lfloor \frac{n}{2} \right\rfloor$.

(ii) If G *is* k*-regular, then* $\nu_i = \sqrt{2k}\vartheta_i$, $i = 1, 2, ..., n$. *Particularly if* $G = K_n$, *then* $\nu_1 = (n-1)\sqrt{2(n-1)}$ *and* $\nu_2 = ... = \nu_n = -\sqrt{2\,(n-1)}$.

(iii) If G *is* $(a, b)-$*semiregular bipartite, then* $\nu_i = \sqrt{a+b}\vartheta_i$, $i = 1, 2, ..., n$. *Also, for* $G = K_{p,q}$ *(*$n = p + q$*),* $\nu_1 = -\nu_n = \sqrt{npq}$ *and* $\nu_2 = ... = \nu_{n-1} = 0$.

Proof.

(i) The proof is clear.

(ii) From [11], if G is k-regular, then $A_N = \sqrt{2k}A$. So $\nu_i = \sqrt{2k}\vartheta_i$, $i = 1, 2, ..., n$. Let $G = K_n$, then the proof is obvious as $\vartheta_1(K_n) = n - 1$ and $\vartheta_2(K_n) = ... = \vartheta_n(K_n) = -1$.

(iii) If G is $(a, b)-$semiregular bipartite, then $A_N = (a + b) A$ yields $\nu_i = \sqrt{a + b}\vartheta_i$, $i = 1, 2, ..., n$. Thinking this fact with $\vartheta_1(K_{p,q}) = -\vartheta_n(K_{p,q}) = \sqrt{pq}$ and $\vartheta_2(K_{p,q}) = ... = \vartheta_{n-1}(K_{p,q}) = 0$ proves (iii).

□

Lemma 5 *Let G be a connected graph of order $n (\geq 2)$, ν_1 be the greatest eigenvalue of A_N and x be the corresponding unit (column) eigenvector. Also, A_N has r $(2 \leq r \leq n)$ distinct eigenvalues iff there exist $r - 1$ real numbers $\nu_1 > \nu_2 > ... > \nu_r$ satisfying*

$$\prod_{i=2}^{r} (A_N - \nu_i I) = \prod_{i=2}^{r} (\nu_1 - \nu_i) x x^T,$$

and $\nu_1 > \nu_2 > ... > \nu_r$ are precisely the r distinct eigenvalues of A_N.

Proof. Clearly A_N is a nonnegative symmetric real matrix and as G is connected it is irreducible. The proof is clear for the matrix A_N by using Theorem 2.1 in [19]. □

Corollary 6 *Let G be a connected graph of order $n (\geq 2)$, then G has two distinct N-eigenvalues iff $G \cong K_n$.*

The diameter of G, $d(G)$, is the maximum distance between any pair of vertices.

Corollary 7 *If G is a connected graph has $t \geq 2$ distinct N-eigenvalues, then $d(G) \leq t - 1$.*

Corollary 8 *A connected bipartite graph G has three distinct N-eigenvalues iff G is complete bipartite.*

The proof of the previous corollaries can be easily seen via Lemma 4 and Lemma 5 by utilizing the results of Theorem 2.1 in [19].

Let $\frac{n}{2}K_2$ be the (disjoint) union of $\frac{n}{2}$ copies of K_2.

Theorem 9 *Let* G *be a graph of order* n*. Then* $|\nu_1| = |\nu_2| = \ldots = |\nu_n|$ *iff* $G \cong \overline{K_n}$ *or* $G \cong \frac{n}{2}K_2$*.*

Proof. Let $|\nu_1| = |\nu_2| = \ldots = |\nu_n|$ and G has m isolated vertices. If $m \geq 1$, then $\nu_1 = \nu_2 = \ldots = \nu_n = 0$. Thus $G \cong \overline{K_n}$. If not, $m = 0$. If $\Delta = 1$, then G is one-regular. So, $G \cong \frac{n}{2}K_2$. If $\Delta \geq 2$, then G has a connected component H of order $k\,(\geq 3)$. From the Perron-Frobenius theorem $\nu_1\,(G) > \nu_2\,(H)$, that is not possible. So, $G \cong \frac{n}{2}K_2$.

Conversely, if $G \cong \overline{K_n}$ or $G \cong \frac{n}{2}K_2$, then proof is clear. □

Lemma 10 ([5]) *Let* G *be a connected graph. Then*

$$\vartheta_1 \leq \sqrt{2e - \delta\,(n-1) + (\delta - 1)\,\Delta}, \tag{1}$$

equality attains in (1) iff G *is regular or a star.*

We are now ready to present our bounds for ν_1.

Corollary 11 *Let* G *be a connected graph. Then*

$$\nu_1 \leq \sqrt{2\Delta\,[2e - \delta\,(n-1) + (\delta - 1)\,\Delta]},$$

where the bound is strict.

Proof. From Lemma 1 and (1), we get

$$\nu_1 \leq \sqrt{2\Delta}\vartheta_1 \leq \sqrt{2\Delta}\sqrt{2e - \delta\,(n-1) + (\delta - 1)\,\Delta}.$$

If G is regular $(\Delta = \delta)$, then using Lemma 10 gives $\nu_1 = \sqrt{2\Delta}\vartheta_1$ namely, the bound is strict. □

Theorem 12 *Let* G *be a graph. Then*

$$\nu_1 \geq \left[\frac{1}{n}\sum_{i=1}^{n}\left(\sum_{i\sim j}(d_i + d_j) + 2\delta\sum_{j\neq i}c_{ij}\right)^2\right]^{1/4}, \tag{2}$$

where $c_{ij} = |N_i \cap N_j|$.

Proof. Considering Rayleigh quotient for real symmetric matrix C with $x = (1, 1, ..., 1)^t$ gives

$$\nu_1^2 \geq \frac{x^t C^2 x}{n} = \frac{(Cx)^t Cx}{n} = \sum_{i=1}^{n} r_i^2 / n \,, \tag{3}$$

where r_i is the i^{th} row sum of C. By Lemma 3, $r_i(A_N^2) = \sum_{i\sim j} (d_i + d_j) + \sum_{i\sim k,\ k\sim j} \sqrt{d_i + d_k}\sqrt{d_k + d_j}$. Then applying (3) to $C = A_N^2$ verifies

$$\begin{aligned}\nu_1 &\geq \left[\frac{1}{n}\sum_{i=1}^{n}\Big(\sum_{i\sim j}(d_i + d_j) + \sum_{i\sim k,\ k\sim j}\sqrt{d_i + d_k}\sqrt{d_k + d_j}\Big)^2\right]^{1/4} \\ &\geq \left[\frac{1}{n}\sum_{i=1}^{n}\Big(\sum_{i\sim j}(d_i + d_j) + \sum_{j\neq i} c_{ij} 2\delta\Big)^2\right]^{1/4},\end{aligned}$$

which leads (2). □

Now, Nordhaus-Gaddum type bound on ν_1 can be followed.

Theorem 13 *Let* G *be a graph. Then*

$$\nu_1 + \overline{\nu_1} \geq \frac{2}{n}\left(2e\sqrt{2\delta} + \left[\binom{n}{2} - e\right]\sqrt{2\,(n - 1 - \Delta)}\right) \tag{4}$$

equality is attained iff G is regular.

Proof. From Lemma 2

$$\nu_1 \geq \frac{2N\,(G)}{n} \geq \frac{2}{n}\sum_{i\sim j}\sqrt{\delta + \delta} = \frac{2e\sqrt{2\delta}}{n}. \tag{5}$$

For any vector $x = (x_1, x_2, ..., x_n)^t \in \mathbb{R}^n$, we get

$$\begin{aligned}x^t\left(A_N + \overline{A_N}\right)x &= x^t A_N x + x^t \overline{A_N} x \\ &= 2\sum_{ij\in E}\sqrt{d_i + d_j}\,x_i x_j + 2\sum_{ij\in E(\overline{G})}\sqrt{\overline{d_i} + \overline{d_j}}\,x_i x_j.\end{aligned} \tag{6}$$

By setting $x = \left(\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, ..., \frac{1}{\sqrt{n}}\right)^t$ in (6) and using (5) provides

$$x^t\left(A_N+\overline{A_N}\right)x = \frac{2}{n}\left[N(G)+N\left(\overline{G}\right)\right] \geq \frac{2}{n}\left(2e\sqrt{2\delta}+\sqrt{2(n-1-\Delta)}\left[\binom{n}{2}-e\right]\right). \tag{7}$$

From Rayleigh-Ritz theorem $\nu_1 \geq x^t A_N x$ and $\overline{\nu_1} \geq x^t \overline{A_N} x$. Using these facts in (7) satisfies the result. Assume that equality attains in (4). So, G is regular. One may simply see that equality holds in (4) when G is regular. □

Now, we suggest bounds for the Nirmala energy. We initially analyze the graph structure attaining the McClelland-type bound (8) given in [11].

Theorem 14 *Let* G *be a graph. Then*

$$En_N(G) \leq \sqrt{2nZg}, \tag{8}$$

equality is attained iff $G \cong \overline{K_n}$ *or* $G \cong \frac{n}{2}K_2$.

Proof. Equality holds in (8) iff $|\nu_1| = |\nu_2| = \ldots = |\nu_n|$. By Theorem 9, $G \cong \overline{K_n}$ or $G \cong \frac{n}{2}K_2$. □

Let we begin to present bounds for $En_N(G)$.

Theorem 15 *Let* G *be a graph. Then*

$$En_N(G) \geq \frac{4e\sqrt{2\delta}}{n}. \tag{9}$$

Proof. Clearly

$$En_N(G) = |\nu_1| + \sum_{i=2}^{n} |\nu_i| \geq |\nu_1| + \left|\sum_{i=2}^{n} \nu_i\right|.$$

As $tr(A_N) = 0$, we have $\nu_1 = -\sum_{i=2}^{n} \nu_i$. Then $|\nu_1| = \left|\sum_{i=2}^{n} \nu_i\right|$, which implies

$$En_N(G) \geq 2|\nu_1| = 2\nu_1.$$

Using (5) results

$$En_N(G) \geq \frac{4e\sqrt{2\delta}}{n}.$$

□

Now, we can give Nordhaus-Gaddum type bound for $En_N(G)$.

Theorem 16 *Let* G *be a connected graph. Then*

$$En_N(G) + En_N(\overline{G}) \geq \frac{4}{n}\left[e\sqrt{2\delta} + \left[\binom{n}{2} - e\right]\sqrt{2(n-1-\Delta)}\right], \qquad (10)$$

the bound is strict.

Proof. By Theorem 15

$$En_N(G) + En_N(\overline{G}) \geq \frac{4}{n}\left[e\sqrt{2\delta} + \overline{e}\sqrt{2\overline{\delta}}\right].$$

So, the inequality (10) is clear as $\overline{e} = \binom{n}{2} - e$ and $\overline{\delta} \geq n - 1 - \Delta$. One may conclude that equality is attained in (10) for complete bipartite regular graphs. □

Let $X \in \mathbb{R}^{n\times n}$ with singular values $\sigma_i(X)$ for $i = 1, 2, ..., n$. If X is symmetric with eigenvalues $\vartheta_i(X)$, then $\sigma_i(X) = |\vartheta_i(X)|$, $i = 1, 2, ..., n$. In [20], the energy $En(X)$ of X is given by $En(X) = \sum_{i=1}^{n} \sigma_i(X)$. This definition allowed the Ky Fan theorem to be applied to studies in graph energy theory [14].

Lemma 17 ([8]) *If* $X, Y \in \mathbb{R}^{n\times n}$ *are symmetric matrices, then*

$$\sum_{i=1}^{n} \sigma_i(X+Y) \leq \sum_{i=1}^{n} \sigma_i(X) + \sum_{i=1}^{n} \sigma_i(Y).$$

Theorem 18 *Let* G *be a graph without isolated vertices, then*

$$En_N(G) \leq 2N(G).$$

Proof. Let G_{uv} be the graph with $V(G_{uv}) = V(G)$ which has only one edge joining the vertices u, v and (i, j)-entry of the Nirmala matrix of G_{uv} be

$$A_N(G_{uv})(i,j) = \begin{cases} \sqrt{d_u + d_v}, & \text{if } (i,j) = (u,v) \text{ or } (j,i) = (u,v) \\ 0, & \text{otherwise.} \end{cases}$$

Thus, the Nirmala matrix of G can be rewritten as

$$A_N(G) = \sum_{uv\in E(G)} A_N(G_{uv}),$$

notice that

$$En(A_N(G_{uv})) = 2\left(\sqrt{d_u + d_v}\right).$$

By repeating the application of Lemma 17, we obtain

$$En_N(G) \leq 2\sum_{u\sim v}\sqrt{d_u+d_v} = 2N(G).$$

□

Theorem 19 *Let* G *be a graph. Then*

$$En_N(G) \leq 2\sqrt{Zg+2\Delta e(e-1)}. \tag{11}$$

Proof. One may get

$$\begin{aligned} N(G)^2 =& \sum_{i\sim j}(d_i+d_j) + \sum_{\substack{i\sim j,\ k\sim t \\ ij\neq kt}}\sqrt{d_i+d_j}\sqrt{d_k+d_t} \\ \leq& Zg+2\Delta e(e-1). \end{aligned}$$

Hence,

$$N(G) \leq \sqrt{Zg+2\Delta e(e-1)}. \tag{12}$$

Using (12) in Theorem 18 leads (11). □

Theorem 20 *Let* G *be a graph. Then*

$$En_N(G) \leq \frac{tr(A_N^3)}{2\delta y}, \tag{13}$$

where $y = \min\{|N_u \cap N_v| : u \sim v\}$.

Proof. Let $\min\{|N_u \cap N_v| : u \sim v\} = y$. By Lemma 3 we have

$$\begin{aligned} tr(A_N^3) =& 2\sum_{i\sim j}\sqrt{d_i+d_j}\sum_{i\sim k,\ k\sim j}\sqrt{d_i+d_k}\sqrt{d_k+d_j} \\ \geq& 4\delta y\sum_{i\sim j}\sqrt{d_i+d_j} \\ =& 4\delta y N(G). \end{aligned}$$

Thus

$$N(G) \leq \frac{tr(A_N^3)}{4\delta y}. \tag{14}$$

Combining Theorem 18 with (14) yields (13). □

Graph energy is expressed as in terms of vertex energies in [1]. Thus

$$\mathrm{En}\,(G) = \sum_{u \in V} \mathrm{En}\,(u)\,.$$

In [2], the energy of a graph is reconsidered as

$$\mathrm{En}\,(G) = \sum_{u \sim v} \frac{\mathrm{En}\,(u)}{d_u} + \frac{\mathrm{En}\,(v)}{d_v}. \tag{15}$$

Lemma 21 ([1]) *Let* G *be a graph with* $e \geq 1$. *Then* $\mathrm{En}\,(u) \geq \sqrt{d_u\,/\Delta}$ *for all* $u \in V$.

Here, we present a bound including graph energy and Δ for $\mathrm{En}_N\,(G)$.

Theorem 22 *Let* G *be a graph with* $e \geq 1$. *Then*

$$\mathrm{En}_N\,(G) \leq 2\Delta^{3/2}\,\mathrm{En}\,(G)\,.$$

Proof. By (15) and Lemma 21

$$\begin{aligned} \mathrm{En}\,(G) &= \sum_{u \sim v} \frac{\mathrm{En}\,(u)}{d_u} + \frac{\mathrm{En}\,(v)}{d_v} \\ &\geq \sum_{u \sim v} \frac{\mathrm{En}\,(u)}{\Delta} + \frac{\mathrm{En}\,(v)}{\Delta} \\ &= \frac{1}{\Delta} \sum_{u \sim v} \mathrm{En}\,(u) + \mathrm{En}\,(v) \\ &\geq \frac{1}{\Delta^{3/2}} \sum_{u \sim v} \sqrt{d_u} + \sqrt{d_v} \\ &\geq \frac{1}{\Delta^{3/2}} \sum_{u \sim v} \sqrt{d_u + d_v} = \frac{N(G)}{\Delta^{3/2}}. \end{aligned} \tag{16}$$

Using (16) and Theorem 18 yields

$$\mathrm{En}\,(G) \geq \frac{\mathrm{En}_N\,(G)}{2\Delta^{3/2}}.$$

□

Lemma 23 *Let* G *be a graph of order* $n\,(\geq 2)$ *has* e *edges. Then* $|\nu_1| = |\nu_2| = ... = |\nu_{p-1}| = |\nu_p| > 0$ $(p \geq 2)$ *and if exists the rest of the N-eigenvalues are* 0 *iff* $G \cong sK_1 \cup \bigcup_{i=1}^{t} K_{\alpha_i,\beta_i}$ *such that* $\sum_{i=1}^{t} (\alpha_i + \beta_i) + s = n$ *with* $t.(\alpha_i.\beta_i) = e$ *for* $i = 1, 2, ..., t$ *and* $p = 2t$.

Proof. Clearly, ν_1 is an N-eigenvalue iff $-\nu_1$ is an N-eigenvalue of G when G is connected. The proof can be seen similar as Lemma 1.3 in [4] by considering Corollary 7-8. □

The following result is clear by setting $p = n$ in Lemma 23.

Corollary 24 *Let* G *be a graph of order* $n\,(\geq 2)$*. Then* $|\nu_1| = |\nu_2| = ... = |\nu_{n-1}| = |\nu_n| > 0$ *iff* $G \cong \frac{n}{2}K_2$.

Lemma 25 ([7]) *Let*$(x_i), (y_i)$ *be decreasing sequences of nonnegative numbers with* $x_1, y_1 \neq 0$ *and* (p_i) *be a sequence of nonnegative numbers for* $i = 1, 2, ..., n$*. Then*

$$\sum_{i=1}^{n} p_i x_i^2 \sum_{i=1}^{n} p_i y_i^2 \leq \max\left\{ y_1 \sum_{i=1}^{n} p_i x_i,\ x_1 \sum_{i=1}^{n} p_i y_i \right\} \sum_{i=1}^{n} p_i x_i y_i. \tag{17}$$

Now we give a new bound on $En_N(G)$ of bipartite graphs.

Theorem 26 *Let* G *be a non-empty bipartite graph of order* $n\,(\geq 2)$*. Then*

$$En_N(G) \geq \frac{2Zg}{\nu_1}, \tag{18}$$

equality holds iff $G \cong \frac{n}{2}K_2$ *or* $G \cong (n - \alpha - \beta)K_1 \cup K_{\alpha,\beta}$.

Proof. Setting $x_i = y_i := |\nu_i|$ and $p_i := 1$ $(1 \leq i \leq n)$ in Lemma 25 and applying (17) gives

$$\sum_{i=1}^{n} |\nu_i|^2 \sum_{i=1}^{n} |\nu_i|^2 \leq \max\left\{ \nu_1 \sum_{i=1}^{n} |\nu_i|, \nu_1 \sum_{i=1}^{n} |\nu_i| \right\} \sum_{i=1}^{n} |\nu_i|^2,$$

hence,

$$\sum_{i=1}^{n} |\nu_i|^2 \leq \nu_1 \sum_{i=1}^{n} |\nu_i|. \tag{19}$$

i.e.,

$$En_N(G) \geq \frac{2Zg}{\nu_1}.$$

Assume that equality holds in (18). Then (19) must be equality, hence $\nu_1 = |\nu_i|$ for all $i \in \{2, ..., n\}$. As G is non-empty, G has at least two distinct N-eigenvalues. Now, two cases can be considered as follows.

(i) The absolute value of all N-eigenvalues are equal.
As G is non-empty graph of order $n\,(\geq 2)$, $\nu_i \neq 0$ for some i. Hence, we have $|\nu_1| = |\nu_2| = ... = |\nu_n| > 0$. Then $G \cong \frac{n}{2}K_2$ from Corollary 24. If $G \cong \frac{n}{2}K_2$, then equality holds.

(ii) The absolute value of all the N-eigenvalues are not equal.
If two N-eigenvalues of G have distinct absolute values, then as G is bipartite we have $\nu_1 = -\nu_n$. So $|\nu_1| = |\nu_n|$, a contradiction. Hence, G has three distinct N-eigenvalues. We have $\nu_1 = -\nu_n \neq 0$ as G is bipartite and $\nu_2 = ... = \nu_{n-1} = 0$. Thus by Lemma 23, $G \cong (n - \alpha - \beta)K_1 \cup K_{\alpha,\beta}$. Conversely, if $G \cong (n - \alpha - \beta)K_1 \cup K_{\alpha,\beta}$, then the equality (18) can be obtained. □

Let we analyze the graph structure attaining the Koolen-Moulton type bound given in [11] for bipartite graphs.

Theorem 27 *Let G be a non-empty bipartite graph of order $n\,(\geq 2)$. Then*

$$En_N(G) \leq \frac{4N(G)}{n} + \sqrt{2(n-2)\left(Zg - 2\left(\frac{2N(G)}{n}\right)^2\right)}, \tag{20}$$

equality holds iff $G \cong \frac{n}{2}K_2$ or $G \cong (n - \alpha - \beta)K_1 \cup K_{\alpha,\beta}$.

Proof. Clearly we have

$$En_N(G) \leq 2\nu_1 + \sqrt{(n-2)\left(2Zg - 2\nu_1^2\right)}.$$

So, the function $h(x) = 2x + \sqrt{(n-2)(2Zg - 2x^2)}$ decreases for $\sqrt{\frac{2Zg}{n}} \leq x \leq \sqrt{2Zg}$. As $\nu_1 \geq \frac{2N(G)}{n} \geq \frac{2}{n}\sqrt{\sum_{i\sim j}(d_i + d_j)} \geq \sqrt{\frac{2Zg}{n}}$, we get $h(\nu_1) \leq h\left(\frac{2N(G)}{n}\right)$ satisfies the equality (20). Suppose that equality holds in (20). Then from the equalities of above arguments give $\nu_1 = -\nu_n = \frac{2N(G)}{n}$ and $|\nu_i| = \sqrt{\frac{2Zg - \nu_1^2}{n-2}}$ for $2 \leq i \leq n-1$. If G is an empty graph, then it has precisely one N-eigenvalue. Thus, G has at least two distinct N-eigenvalues as G is non-empty. So, two cases can be followed:

(i) The absolute value of all N-eigenvalues are equal.

As G is non-empty graph of order $n\,(\geq 2)$, $\nu_i \neq 0$ for some i. Hence, we have $|\nu_1| = |\nu_2| = \ldots = |\nu_n| > 0$. So $G \cong \frac{n}{2}K_2$ from Corollary 24. If $G \cong \frac{n}{2}K_2$, then equality holds.

(ii) The absolute value of all the N-eigenvalues are not equal.

If two N-eigenvalues of G have distinct absolute values, then as G is bipartite we have $\nu_1 = -\nu_n$. So $|\nu_1| = |\nu_n|$, a contradiction. Hence, G has three distinct N-eigenvalues. We have $\nu_1 = -\nu_n \neq 0$ as G is bipartite. Then $\nu_2 = \ldots = \nu_{n-1} = 0$ as $tr(A_{N)} = 0$. Thus, by Lemma 23, $G \cong (n-\alpha-\beta)K_1 \cup K_{\alpha,\beta}$, $\alpha+\beta \leq n$. Conversely, if $G \cong (n-\alpha-\beta)K_1 \cup K_{\alpha,\beta}$, then the equality (20) can be easily followed. □

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