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Some bounds on the A_α-energy of graphs

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Abstract. Let G be a graph with order n and size m. For any real number $\alpha \in [0, 1]$, Nikiforov defined the matrix $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$, where $A(G)$ is the adjacency matrix and $D(G)$ is the diagonal matrix of the vertex degrees. Let ρ_i $(i = 1, 2, \ldots, n)$ denote the eigenvalues of $A_\alpha(G)$ and $E^{A_\alpha}(G) = \sum_{i=1}^{n} |\rho_i - \frac{2\alpha m}{n}|$ denote the A_α-energy of G. In this paper, we get some lower bounds of $E^{A_\alpha}(G)$ in terms of the order, the size and the first Zagreb index of G for $\alpha \in [\frac{1}{2}, 1)$, and characterize the extremal graphs when attaining the bounds if G is regular. In addition, we give some lower and upper bounds of $E^{A_\alpha}(G)$ under the condition that $\rho_1 + \rho_n \geq \frac{4\alpha m}{n}$.

1. Introduction

All graphs considered in this paper are simple and undirected. Let $G = (V, E)$ be a graph with order n and size m, where $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let d_i denote the degree of a vertex v_i in G. Let $\Delta(G)$ and $\delta(G)$ be the maximum and the minimum degree of G, respectively. The first Zagreb index is defined as $M_1 = \sum_{u \in V(G)} d_G^2(u)$. The adjacency matrix $A(G) = (a_{ij})_{n\times n}$ of G is a symmetric $(0, 1)$-matrix of order n, where $a_{ij} = 1$ if v_i is adjacent to v_j; and $a_{ij} = 0$ otherwise. The Laplacian matrix and the signless Laplacian matrix (also known as the Q-matrix) are $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$, respectively, where $D(G)$ is the diagonal matrix of vertex degrees. For any real number $\alpha \in [0, 1]$, Nikiforov [12] defined the matrix $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$, which is a convex combination of $A(G)$ and $D(G)$. The A_α-spectral radius of G, denoted by ρ, is the maximum eigenvalue of $A_\alpha(G)$. The study of the A_α-spectra has received a lot of attention of researchers in recent years (see e.g., [9, 10]); and our team considered the A_α-spectral radius of a graph G with given parameters (see e.g., [7, 8]). However, there are few studies on the A_α-energy so far.

Gutman [5] defined the energy of a graph G as the sum of absolute values of adjacency eigenvalues of G. In the past few decades, the study of energy of graphs has attracted the interest of many scholars. Nikiforov [13] showed that graphs that are close to regular can be made regular with a negligible change of the energy. Also a k-regular graph can be extended to a k-regular graph of a slightly larger order with almost the same energy. Consequently, Gutman and Zhou [6] introduced the conception of Laplacian energy $E^L(G) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}|$, and Ganie and Pirzada [3] proposed signless Laplacian energy $E^Q(G) = \sum_{i=1}^{n} |q_i - \frac{2m}{n}|$,

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where μ_i and q_i $(1 \leq i \leq n)$ are the Laplacian and the signless Laplacian eigenvalues of G, respectively. There are lots of results about $E^L(G)$ and $E^Q(G)$ in terms of the order, the size and the first Zagreb index; see e.g., [3, 15].

Gou and Zhou [4] defined the A_α-energy of a graph G as $E^{A_\alpha}(G) = \sum_{i=1}^{n} |\rho_i - \frac{2\alpha m}{n}|$. Our motivation comes from Wang and Huang [17], in which the authors gave two lower and one upper bounds of Q-energy of graph G and characterized the extremal graphs when attaining the bounds. In this paper, we shall give some lower and upper bounds of $E^{A_\alpha}(G)$ in terms of the order, the size and the first Zagreb index of a graph G.

Let $\gamma_i = |\rho_i - \frac{2\alpha m}{n}|$, thus $E^{A_\alpha}(G) = \sum_{i=1}^{n} \gamma_i$. Set γ_i in a non-decreasing order $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n \geq 0$. We know that once each of $\gamma_i > 0$, $i = 1, 2, \ldots, n$, it has contribution to the $E^{A_\alpha}(G)$. So we usually assume $\gamma_n > 0$, and in this circumstance, we get Theorem 1.1 and characterize the extremal graphs. However, if $\gamma_n = 0$, which means that the corresponding eigenvalue equals $\frac{2\alpha m}{n}$, such as the complete bipartite graphs, the bound given in Theorem 1.1 is 0, and consequently, we give a lower bound for these classes of graphs in Theorem 1.2. Throughout the paper, we use K_n to denote the complete graph of order n, C_n the cycle of order n and K_{n_1,n_2} the complete bipartite graph with order $n = n_1 + n_2$.

Theorem 1.1. *Let G be a graph with n vertices and m edges, M_1 be the first Zagreb index. If $\alpha \in [\frac{1}{2}, 1)$ and $\gamma_n > 0$, then*

$$E^{A_\alpha}(G) \geq 2\sqrt{[2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}]n} \cdot \frac{\sqrt{\gamma_1 \gamma_n}}{\gamma_1 + \gamma_n}, \tag{1.1}$$

where $E^{A_\alpha}(G) = \sum_{i=1}^{n} \gamma_i$ and $\gamma_i = |\rho_i - \frac{2\alpha m}{n}|$.

Especially, if G is a regular graph, the equality holds if and only if $G \cong \frac{n}{2}K_2$ or $gK_{\frac{2m}{n}+1} \bigcup h(K_{\frac{2m}{n}+1,\frac{2m}{n}+1} \backslash F)$, where g and h are some non-negative integers, $\frac{2m}{n} \geq 2$ is an integer, F is a perfect matching of $K_{\frac{2m}{n}+1,\frac{2m}{n}+1}$.

Set $\gamma_n = 0$, the following Theorem 1.2 can be obtained immediately.

Theorem 1.2. *Let G be a connected graph with n vertices and m edges, M_1 be the first Zagreb index. If $\alpha \in [\frac{1}{2}, 1)$ and $\gamma_n = 0$, then*

$$E^{A_\alpha}(G) \geq \frac{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}}{\gamma_1}, \tag{1.2}$$

the equality holds if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

The rest of the paper is organized as follows. In Section 2, we present the proof of Theorem 1.1 and Theorem 1.2. In Section 3, we give some lower and upper bounds of $E^{A_\alpha}(G)$ under the condition that $\rho_1 + \rho_n \geq \frac{4\alpha m}{n}$.

2. Proof of Theorem 1.1 and Theorem 1.2

Firstly, we will give some tools which are used to prove Theorem 1.1. Note that

$$\begin{cases} \sum_{i=1}^{n} \rho_i = 2\alpha m & (2.1) \\ \sum_{i=1}^{n} \rho_i^2 = 2(1-\alpha)^2 m + \alpha^2 M_1. & (2.2) \end{cases}$$

Lemma 2.1. *Let G be a connected r-regular graph with n vertices, m edges and $\alpha \in [0, 1]$.*

(1) *If G is a bipartite graph and $Spec_{A_\alpha}(G) = \{r, [\alpha(r+1)-1]^a, [\alpha(r-1)+1]^b, (2\alpha-1)r\}$, then $a = b = r = \frac{n}{2} - 1$ and $G \cong K_{r+1,r+1} \backslash F$, where F is a perfect matching of the bipartite graph $K_{r+1,r+1}$.*
(2) *If G is a bipartite graph and $Spec_{A_\alpha}(G) = \{r, [r(2\alpha-1)]^a, [\alpha r]^b\}$, then $a = 1$, $b = n-2$, $r = n-1$ and $G \cong K_{\frac{n}{2},\frac{n}{2}}$.*

(3) If $Spec_{A_\alpha}(G) = \{r, [\alpha(r-1)+1]^a, [\alpha(r+1)-1]^b\}$, *then* $a = 0$, $b = r = n-1$ *and* $G \cong K_{r+1}$.

Proof. (1) By equations (2.1) and (2.2), we have

$$\begin{cases} r + a[\alpha(r+1)-1] + b[\alpha(r-1)+1] + r(2\alpha-1) = 2\alpha m, \\ r^2 + a[\alpha(r+1)-1]^2 + b[\alpha(r-1)+1]^2 + [r(2\alpha-1)]^2 = 2(1-\alpha)^2 m + \alpha^2 M_1. \end{cases}$$

Since $n = 2 + a + b$ and $m = \frac{nr}{2}$, $a = b = r = \frac{n}{2} - 1$. Then $G \cong K_{r+1,r+1} \backslash F$ since G is a connected r-regular bipartite graph, where F is a perfect matching of the bipartite graph $K_{r+1,r+1}$. The proof of (2) and (3) are similar to (1). □

Lemma 2.2. [16] Let G be a connected graph with three distinct A_α-eigenvalues $\rho_1 > \rho_2 > \rho_3$ and vertex set $\{v_1, \ldots, v_n\}$. Let d_i denote the degree of vertex v_i. Then there exists the Perron-Frobenius eigenvector $u^T = (u_1, \ldots, u_n)$ such that

(1) $(A_\alpha(G) - \rho_2 I_n)(A_\alpha(G) - \rho_3 I_n) = uu^T$;

(2) $\alpha^2 d_i^2 + \beta^2 d_i - (\rho_2 + \rho_3)\alpha d_i + \rho_2\rho_3 = u_i^2$;

(3) $\alpha\beta(d_i + d_j) + \beta^2\lambda_{ij} - \beta(\rho_2 + \rho_3) = u_i u_j$, where λ_{ij} is the number of common neighbors of two adjacent vertices v_i and v_j;

(4) $\beta^2\mu_{ij} = u_i u_j$, where μ_{ij} is the number of common neighbors of two nonadjacent vertices v_i and v_j and $\beta = 1 - \alpha$.

Let $m_\rho(G)$ be the multiplicity of the A_α-eigenvalues of G.

Lemma 2.3. *Let* G *be an* r*-regular graph,* $\alpha \in [\frac{1}{2}, 1)$*, then* $m_{r(2\alpha-1)}(G)$ *equals the number of the components that are bipartite.*

Proof. Let u *be the eigenvector of the* $Q(G)$ *corresponding to eigenvalue* 0*, it is obvious that*

$$A_\alpha(G) = (2\alpha-1)D(G) + (1-\alpha)Q(G).$$

If $\alpha \in [\frac{1}{2}, 1)$*, then*

$$\left(\frac{A_\alpha(G)}{1-\alpha} - \frac{2\alpha-1}{1-\alpha}D(G)\right)u = Q(G)u = 0.$$

By simple calculation, we obtain that

$$A_\alpha(G)u = r(2\alpha-1)I_{n\times n}u.$$

Thus, $r(2\alpha-1) \in Spec_{A_\alpha}(G)$*. Note that the multiplicity of eigenvalue* 0 *of* $Q(G)$ *equals the number of the components that are bipartite, therefore,* $m_{r(2\alpha-1)}(G)$ *equals the number of the components that are bipartite.* □

Lemma 2.4. [16] A connected regular graph G with three distinct A_α-eigenvalues is a strongly regular graph.

Lemma 2.5. *Let* G *be a non-connected* r*-regular graph with* n *vertices and* m *edges,* $\alpha \in [\frac{1}{2}, 1)$*. If*

$$Spec_{A_\alpha}(G) = \{[r]^{s'}, [r(2\alpha-1)]^{s-s'}, [\alpha(r-1)+1]^a, [\alpha(r+1)-1]^b\},$$

where a*,* b*,* s*,* s' *are nonnegative integers such that* $n = s + a + b$ *and* $s > s' > 1$*, then* $G \cong gK_{r+1} \bigcup h(K_{r+1,r+1}\backslash F)$*, and* $a = r(s-s')$*,* $b = rs'$*,* $r = \frac{n}{s} - 1 \geq 2$*,* $g = 2s' - s$*,* $h = s - s'$*, where* F *is a perfect matching of the bipartite graph* $K_{r+1,r+1}$*.*

Proof. *Since $n = s + a + b$ and $m = \frac{nr}{2}$, $a = r(s - s')$, $b = rs'$ and $r = \frac{n}{s} - 1$ by equations* (2.1) *and* (2.2). *Note that G is a non-connected r-regular graph, then G has exactly s' connected components since $m_r(G) = s'$. Let G_i be the connected components of G with order n_i and size m_i for $1 \le i \le s'$, clearly, $n = \sum_{i=1}^{s'} n_i$ and $m = \sum_{i=1}^{s'} m_i$. If $r(2\alpha - 1) \notin Spec_{A_\alpha}(G_i)$, then*

$$Spec_{A_\alpha}(G_i) = \{r, [\alpha(r-1)+1]^{a_i}, [\alpha(r+1)-1]^{b_i}\}, \tag{2.3}$$

where $0 \le a_i \le a$ and $0 \le b_i \le b$. Then $G_i \cong K_{r+1}$, and $a_i = 0$, $b_i = r = n_i - 1$ by (3) of Lemma 2.1. If $r(2\alpha - 1) \in Spec_{A_\alpha}(G_i)$ and $m_{(r(2\alpha-1))}(G_i) = s_i$, then the A_α-spectra of G has the following four cases.
Case 1. *$Spec_{A_\alpha}(G_i) = \{r, [r(2\alpha - 1)]^{n-1}\}$. Then $r = 1$ and $\alpha = \frac{1}{2}$ by equations* (2.1) *and* (2.2)*, a contradiction.*
Case 2. *$Spec_{A_\alpha}(G_i) = \{r, [(2\alpha - 1)r]^{s_i}, [\alpha(r-1)+1]^{a_i}\}$. Then G is a strongly regular graph by Lemma 2.4 and $u_i = 0$ by (2) of Lemma 2.2, it contradicts with the truth that u_i is Perron-Frobenius vector.*
Case 3. *$Spec_{A_\alpha}(G_i) = \{r, [(2\alpha - 1)r]^{s_i}, [\alpha(r+1)-1]^{b_i}\}$. Then $r = 0$ or $r = \frac{2\alpha s_i - n_i - s_i + 1}{2\alpha s_i - s_i - 1}$ by equations* (2.1) *and* (2.2)*. It's obvious that $r = 0$ is impossible. Since G_i has three distinct A_α-eigenvalues, $r = \frac{2\alpha s_i - n_i - s_i + 1}{2\alpha s_i - s_i - 1} \ge 2$ and $n_i \ge 3$. However, $(2\alpha s_i - n_i - s_i + 1) - (2\alpha s_i - s_i - 1) = -n_i + 2 < 0$, thus, $r \le 1$, a contradiction.*
Case 4.

$$Spec_{A_\alpha}(G_i) = \{r, [(2\alpha - 1)r]^{s_i}, [\alpha(r-1)+1]^{a_i}, [\alpha(r+1)-1]^{b_i}\}. \tag{2.4}$$

Clearly, $s_i = 1$. Then $G_i \cong K_{r+1,r+1} \backslash F$ and $a_i = b_i = r$ by Lemma 2.3 and (1) of Lemma 2.1.

By the above discussion, $G \cong gK_{r+1} \bigcup h(K_{r+1,r+1} \backslash F)$, where $r \ge 2$, $g = 2s' - s$ and $h = s - s'$. In (2.3)*, $b_j = r$ for $1 \le j \le g$; In* (2.4)*, $s_i = 1$ and $a_i = b_i = r$ for $g + 1 \le i \le g + h$. Analyzing the A_α-spectra, we have $g + h = s'$, $s_i h = s - s'$, $a_i h = a$ and $b_i h + b_j g = b$. Therefore, $h = \frac{a}{r} = s - s'$ and $g = s' - h = 2s' - s$.* □

Lemma 2.6. [12] Let G be a simple graph with n vertices and m edges, ρ_1 be the largest A_α-eigenvalue. Then $\rho_1 \ge \frac{2m}{n}$, the equality holds if and only if G is a regular graph.

Lemma 2.7. [14] Let $n \ge 1$ be an integer and $a_1 \ge a_2 \ge \cdots \ge a_n$ be some non-negative real numbers. Then $\sum_{i=1}^{n} a_i(a_1 + a_n) \ge \sum_{i=1}^{n} a_i^2 + n a_1 a_n$, the equality holds if and only if $a_1 = a_2 = \cdots = a_s$ and $a_{s+1} = \cdots = a_n$ for $s \in \{1, \ldots, n\}$.

Note that a connected regular graph G with just two distinct A_α-eigenvalues is a complete graph.

Proof of Theorem 1.1.

Proof. According to equations (2.1) and (2.2), we have

$$\begin{aligned}\sum\nolimits_{i=1}^{n} \gamma_i^2 &= \sum\nolimits_{i=1}^{n} |\rho_i - \frac{2\alpha m}{n}|^2 \\ &= \sum\nolimits_{i=1}^{n} |\rho_i|^2 - \frac{4\alpha m}{n} \sum\nolimits_{i=1}^{n} \rho_i + \sum\nolimits_{i=1}^{n} (\frac{2\alpha m}{n})^2 \\ &= 2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}.\end{aligned} \tag{2.5}$$

By Lemma 2.7, we have

$$
\begin{aligned}
E^{A_\alpha}(G)=\sum\nolimits_{i=1}^{n}\gamma_i &\geq \frac{\sum_{i=1}^{n}{\gamma_i}^2+n\gamma_1\gamma_n}{\gamma_1+\gamma_n}\\
&=\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}+n\gamma_1\gamma_n}{\gamma_1+\gamma_n}\\
&\geq \frac{2\sqrt{[2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}]n\gamma_1\gamma_n}}{\gamma_1+\gamma_n}\\
&=2\sqrt{[2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}]n}\cdot\frac{\sqrt{\gamma_1\gamma_n}}{\gamma_1+\gamma_n},
\end{aligned}
$$

the equality holds if and only if $\gamma_1=\cdots=\gamma_s$, $\gamma_{s+1}=\cdots=\gamma_n$ for $1\leq s\leq n$ and $2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}=n\gamma_1\gamma_n$. Let $\gamma_1=\cdots=\gamma_s=\tau\geq\gamma_{s+1}=\cdots=\gamma_n=\varphi>0$, then

$$2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}=n\tau\varphi>0, \tag{2.6}$$

and we have $s\tau^2+(n-s)\varphi^2=n\tau\varphi$ by (2.5) and (2.6), then

$$s(\tau+\varphi)(\tau-\varphi)=n\varphi(\tau-\varphi). \tag{2.7}$$

If G is regualar, then we have the following two situations for the above equations.
Case 1. $\tau=\varphi$. Then $|\rho_i-\frac{2\alpha m}{n}|=\gamma_i=\tau$, and $Spec_{A_\alpha}(G)=\{[\tau+\frac{2\alpha m}{n}]^a,[-\tau+\frac{2\alpha m}{n}]^b\}$, where $a+b=n$. Combining with $(a-b)\tau=0$ by equation (2.1). Thus, $\tau=0$ or $a=b$ ($\tau\neq 0$). Since $\tau>0$, $a=b$. Then $Spec_{A_\alpha}(G)=\{[\tau+\frac{2\alpha m}{n}]^{\frac{n}{2}},[-\tau+\frac{2\alpha m}{n}]^{\frac{n}{2}}\}$. Obviously, $\rho_1=\tau+\frac{2\alpha m}{n}$ is the A_α-spectral radius of G. If $n=2$, then ρ_1 is simple and $G=K_2$. If $n>2$, then G is non-connected by Perron-Frobenius Theorem, let G_1 be one of the connected components of G which has A_α-spectral radius $\rho_1=\tau+\frac{2\alpha m}{n}$, then G has $\frac{n}{2}$ connected components exactly, denoted by $G_1,\ldots,G_{\frac{n}{2}}$ and $Spec_{A_\alpha}(G_i)=\{[\tau+\frac{2\alpha m}{n}]^1,[-\tau+\frac{2\alpha m}{n}]^1\}$. Then $G_i=K_2$ and $G\cong\frac{n}{2}K_2$.
Case 2. $\tau\neq\varphi$. Then there exists $1\leq s<n$ such that $|\rho_i-\frac{2\alpha m}{n}|=\gamma_i=\tau$ for $i=1,\ldots,s$ and $|\rho_j-\frac{2\alpha m}{n}|=\gamma_j=\varphi$ for $j=s+1,\ldots,n$, then

$$Spec_{A_\alpha}(G)=\{[\tau+\frac{2\alpha m}{n}]^{s'},[\varphi+\frac{2\alpha m}{n}]^{a},[-\tau+\frac{2\alpha m}{n}]^{s-s'},[-\varphi+\frac{2\alpha m}{n}]^{b}\}, \tag{2.8}$$

where $a+b=n-s$. Clearly, $\tau+\frac{2\alpha m}{n}>\varphi+\frac{2\alpha m}{n}>-\varphi+\frac{2\alpha m}{n}>-\tau+\frac{2\alpha m}{n}$ and $\rho_1=\tau+\frac{2\alpha m}{n}$ is the A_α-spectral radius of G. Since $\rho_1=\frac{2m}{n}$ by Lemma 2.6, we can conclude that $\tau=\frac{2(1-\alpha)m}{n}$.
Subcase 2.1. G is a connected graph. Then $s'=1$ and ρ_1 is simple. If $s\geq 2$, then $\rho_i=-\tau+\frac{2\alpha m}{n}$ for $i=2,3,\ldots,s$. Since $\tau=\frac{2(1-\alpha)m}{n}$, $\rho_1=\frac{2m}{n}$, and G is a $\frac{2m}{n}$-regular graph by Lemma 2.6. Thus, $\varphi=1-\alpha$ by (2.6), and $Spec_{A_\alpha}(G)=\{\frac{2m}{n},[\frac{2(2\alpha-1)m}{n}]^{s-1},[\frac{2\alpha m}{n}+(1-\alpha)]^a,[\frac{2\alpha m}{n}-(1-\alpha)]^b\}$, where $n=s+a+b$. Since G is connected and combining with Lemma 2.3, G is a bipartite graph and $s=2$, then $G\cong K_{\frac{2m}{n}+1,\frac{2m}{n}+1}\backslash F$ by (1) of Lemma 2.1. If $s=1$, $\varphi=1-\alpha$ as before, then $Spec_{A_\alpha}(G)=\{\frac{2\alpha m}{n}+\frac{2(1-\alpha)m}{n},[\frac{2\alpha m}{n}+1-\alpha]^a,[\frac{2\alpha m}{n}-(1-\alpha)]^b\}$, where $a+b=n-1$ and $G\cong K_{\frac{2m}{n}+1}$ by (3) of Lemma 2.1.

Hence, $G\cong K_{\frac{2m}{n}+1}$ or $G\cong K_{\frac{2m}{n}+1,\frac{2m}{n}+1}\backslash F$ if G is connected.
Subcase 2.2. G is a non-connected graph. $Spec_{A_\alpha}(G)=\{[\frac{2m}{n}]^{s'},[\frac{2(2\alpha-1)m}{n}]^{s-s'},[\frac{2\alpha m}{n}+(1-\alpha)]^a,[\frac{2\alpha m}{n}-(1-\alpha)]^b\}$, it's same as the above discussion, thus $G\cong gK_{\frac{2m}{n}+1}\cup h(K_{\frac{2m}{n}+1,\frac{2m}{n}+1}\backslash F)$ by Lemma 2.5, where $\frac{2m}{n}\geq 2$ is an integer, $g=2s'-s$ and $h=s-s'$. Then we have completed the proof. □

For two vertex disjoint graphs G and H, we denote $G\vee H$ the join of G and H.

Remark 2.8. *Underlying the condition of proving the equality's holding of Theorem 1.1, if G is irregular, then $\tau > \frac{2(1-\alpha)m}{n}$ and we have the following two cases.*

Case 1. *G is connected. Then $s' = 1$ and $Spec_{A_\alpha}(G) = \{[\tau + \frac{2\alpha m}{n}]^{s'}, [\varphi + \frac{2\alpha m}{n}]^{a}, [-\tau + \frac{2\alpha m}{n}]^{s-s'}, [-\varphi + \frac{2\alpha m}{n}]^{b}\}$ with the condition that $\tau \geq \varphi > 0$, then $\tau + \frac{2\alpha m}{n} \geq \varphi + \frac{2\alpha m}{n} > -\varphi + \frac{2\alpha m}{n} \geq -\tau + \frac{2\alpha m}{n}$. If $\tau = \varphi$, then $Spec_{A_\alpha}(G) = \{[\tau + \frac{2\alpha m}{n}]^{1}, [\tau + \frac{2\alpha m}{n}]^{a}, [-\tau + \frac{2\alpha m}{n}]^{s-s'}, [-\tau + \frac{2\alpha m}{n}]^{b}\}$. Due to G is connected, then $a = 0$ and $Spec_{A_\alpha}(G) = \{[\tau + \frac{2\alpha m}{n}]^{1}, [-\tau + \frac{2\alpha m}{n}]^{n-1}\}$, consequently, $G \cong K_n$, it contradicts with G is irregular. If $\tau \neq \varphi$, then $\tau + \frac{2\alpha m}{n} > \varphi + \frac{2\alpha m}{n} > -\varphi + \frac{2\alpha m}{n} > -\tau + \frac{2\alpha m}{n}$, and we have $(2s' - s)\tau = (b - a)\varphi$ by equation (2.1). If $s = 2$, then $a = b$ or $\varphi = 0$. Since $\varphi > 0$, $a = b$. Then $Spec_{A_\alpha}(G) = \{\tau + \frac{2\alpha m}{n}, [\varphi + \frac{2\alpha m}{n}]^{\frac{n}{2}-1}, -\tau + \frac{2\alpha m}{n}, [-\varphi + \frac{2\alpha m}{n}]^{\frac{n}{2}-1}\}$, in addition, $\tau + \frac{2\alpha m}{n} > \frac{2m}{n}$ and $-\tau + \frac{2\alpha m}{n} < \frac{2(2\alpha-1)m}{n}$. It is a pity that we can't characterize the extremal graph absolutely, however, after doing a series of calculations by MATLAB and Mathematica, we obtain some graphs satisfying the A_α-spectra that $\tau + \frac{2\alpha m}{n} > \varphi + \frac{2\alpha m}{n} > -\varphi + \frac{2\alpha m}{n} > -\tau + \frac{2\alpha m}{n}$ ($\rho_1 > \rho_2 > \rho_3 > \rho_4$) which are listed as follows:*

Table 1:

Graph	P_4, $\alpha \in [\frac{1}{2}, 1)$	$K_2 \vee 2K_1$, $\alpha \in [\frac{10-\sqrt{5}}{10}, 1)$
ρ_1	$\frac{\sqrt{4\alpha^2-8\alpha+5}+2\alpha+1}{2}$	$4\alpha - 1$
ρ_2	$\frac{\sqrt{8\alpha^2-12\alpha+5}+4\alpha-1}{2}$	$\frac{\sqrt{16\alpha^2-32\alpha+17}+4\alpha+1}{2}$
ρ_3	$\frac{2\alpha+1-\sqrt{4\alpha^2-8\alpha+5}}{2}$	2α
ρ_4	$\frac{4\alpha-1-\sqrt{8\alpha^2-12\alpha+5}}{2}$	$\frac{4\alpha+1-\sqrt{16\alpha^2-32\alpha+17}}{2}$

If $s > 2$, then we obtain graphs as $s = 2$ and $a = b$. If $s = 1$, then $Spec_{A_\alpha}(G) = \{\frac{2\alpha m}{n} + \tau, [\frac{2\alpha m}{n} + \varphi]^{a}, [\frac{2\alpha m}{n} - \varphi]^{b}\}$, where $a + b = n - 1$, $\tau > \frac{2(1-\alpha)m}{n}$ and $0 < \varphi < \frac{2\alpha m}{n}$. Thus $\tau = (n-1)\varphi$ by (2.7) and $2a\varphi = 0$ by equation (2.1). Since $\varphi > 0$, $a = 0$. Thus, G has two different A_α-eigenvalues and $G \cong K_n$. It contradicts with G is irregular.

Case 2. *G is non-connected. $Spec_{A_\alpha}(G) = \{[\tau + \frac{2\alpha m}{n}]^{s'}, [\varphi + \frac{2\alpha m}{n}]^{a}, [-\tau + \frac{2\alpha m}{n}]^{s-s'}, [-\varphi + \frac{2\alpha m}{n}]^{b}\}$. We have $s' \geq 1$, $\tau > \frac{2(1-\alpha)m}{n}$, $0 < \varphi \leq \frac{2\alpha m}{n}$, $\tau = \frac{n-s}{s}\varphi$ by (2.7) and $(2s' - s)\tau = (b - a)\varphi$ by equation (2.1). It is a pity that we can't characterize the extremal graph.*

Lemma 2.9. [18] Let G be a connected graph of order $n \geq 3$. Then $m_\rho(G) = n - 2$ if and only if

(1) $G \cong K_{1,n-1}$, or

(2) $G \cong K_{\frac{n}{2},\frac{n}{2}}$ with $n \geq 4$, or

(3) $G \cong K_s \vee (n-s)K_1$ with $2 \leq s \leq n-2$ and $\alpha = \frac{1}{n-s}$, or

(4) $G \cong K_1 \vee K_{\frac{n-1}{2},\frac{n-1}{2}}$ with $n \geq 5$ and $\alpha = \frac{4}{n+1}$, or

(5) $G \cong sK_1 \vee (K_1 \cup K_{n-s-1})$ with $s \geq 3$, $n = 3s - 2$ and $\alpha = \frac{3}{n-1}$, or

(6) $G \cong K_1 \vee 2K_{\frac{n-1}{2}}$ with $n \geq 5$ and $\alpha = \frac{2}{n+1}$.

For convenience, the A_α-spectra of the above graphs are shown in the following table.

Table 2: The A_α-spectra of graphs

Graphs	A_α-spectra
$K_{1,n-1}$	$\{\frac{n\alpha+\sqrt{(n\alpha)^2+4(n-1)(1-\alpha)}}{2},[\alpha]^{n-2},\frac{n\alpha-\sqrt{(n\alpha)^2+4(n-1)(1-\alpha)}}{2}\}$
$K_{\frac{n}{2},\frac{n}{2}}$	$\{\frac{n}{2},[\frac{n\alpha}{2}]^{n-2},\frac{n(2\alpha-1)}{2}\}$
$K_s\vee(n-s)K_1,(\alpha=\frac{1}{n-s})$	$\{\frac{ns+s-s^2+(n-s-1)\sqrt{s(4n-3s)}}{2(n-s)},[\frac{s}{n-s}]^{n-2},\frac{ns+s-s^2-(n-s-1)\sqrt{s(4n-3s)}}{2(n-s)}\}$
$K_1\vee K_{\frac{n-1}{2},\frac{n-1}{2}},(\alpha=\frac{4}{n+1})$	$\{\frac{n^2+4n-5}{2(n+1)},[2]^{n-2},\frac{-n^2+8n+1}{2(n+1)}\}$
$sK_1\vee(K_1\cup K_{2s-3}),(\alpha=\frac{3}{n-1})$	$\{\frac{s^2-2s+2+(s-2)\sqrt{(3s-1)(s-1)}}{s-1},[2]^{n-2},\frac{s^2-2s+2-(s-2)\sqrt{(3s-1)(s-1)}}{s-1}\}$
$K_1\vee 2K_{\frac{n-1}{2}},(\alpha=\frac{2}{n+1})$	$\{\frac{(n-1)^2}{2(n+1)},\frac{n^2+2n-3}{2(n+1)},[0]^{n-2}\}$

Proof of Theorem 1.2.

Proof. By Lemma 2.7, (2.5) and $\gamma_n = 0$, we have

$$E^{A_\alpha}(G) \geq \frac{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}}{\gamma_1},$$

the equality holds if and only if $\gamma_1 = \cdots = \gamma_s$ and $\gamma_{s+1} = \cdots = \gamma_n = 0$ for $1 \leq s \leq n$.

If the equality in (1.2) holds, then there exists $1 \leq s \leq n$ such that $\gamma_i = |\rho_i - \frac{2\alpha m}{n}| = \tau$ for $i = 1, 2, \ldots, s$ and $\gamma_j = |\rho_i - \frac{2\alpha m}{n}| = 0$ for $j = s+1, \ldots, n$. We have $Spec_{A_\alpha}(G) = \{[\tau + \frac{2\alpha m}{n}]^{s'}, [\frac{2\alpha m}{n} - \tau]^{s-s'}, [\frac{2\alpha m}{n}]^{n-s}\}$ and $\tau + \frac{2\alpha m}{n} > \frac{2\alpha m}{n} > \frac{2\alpha m}{n} - \tau$ for $\tau > 0$, then $\rho_1 = \tau + \frac{2\alpha m}{n}$ is the A_α-spectral radius of G . Due to G is a connected graph, then

$$Spec_{A_\alpha}(G) = \{\tau + \frac{2\alpha m}{n}, [\frac{2\alpha m}{n} - \tau]^{s-1}, [\frac{2\alpha m}{n}]^{n-s}\}. \tag{2.9}$$

Since $\rho_1 \geq \frac{2m}{n}$ by Lemma 2.6, $\tau \geq \frac{2(1-\alpha)m}{n}$.

If G is a connected r-regular graph, then $\tau = \frac{2(1-\alpha)m}{n} = (1-\alpha)r$, and $Spec_{A_\alpha}(G) = \{r, [\alpha r]^{n-s}, [(2\alpha-1)r]^{s-1}\}$ by (2.9). We have $s = 2$, $r = \frac{n}{2}$ by equations (2.1) and (2.2). Then $Spec_{A_\alpha}(G) = \{\frac{n}{2}, \frac{(2\alpha-1)n}{2}, [\frac{\alpha n}{2}]^{n-2}\}$ and $G \cong K_{\frac{n}{2},\frac{n}{2}}$ by Lemma 2.3 and (2) of Lemma 2.1.

If G is an irregular graph, then $\tau > \frac{2(1-\alpha)m}{n}$ by Lemma 2.6. And $(2-s)\tau = 0$ by equation (2.1) since $\tau > \frac{2(1-\alpha)m}{n} \neq 0$, $s = 2$. Then $Spec_{A_\alpha}(G) = \{\tau + \frac{2\alpha m}{n}, \frac{2\alpha m}{n} - \tau, [\frac{2\alpha m}{n}]^{n-2}\}$. We are supposed to consider the following situations by Lemma 2.9.

(1) If $G = K_{1,n-1}$, we have $\frac{2m\alpha}{n} = \frac{2(n-1)\alpha}{n} = \alpha$, then $n = 2$, it contradicts with $n \geq 3$.

(2) If $G = K_{\frac{n}{2},\frac{n}{2}}$, then it contradicts with G is an irregular graph.

(3) If $G = K_s \vee (n-s)K_1$ and $\alpha = \frac{1}{n-s}$, then $s > s$, a contradiction.

(4) If $G = K_1 \vee K_{\frac{n-1}{2},\frac{n-1}{2}}$ and $\alpha = \frac{4}{n+1}$, then $n = 3$, which means that $G \cong C_3$, it contradicts with G is an irregular graph.

(5) If $G = sK_1 \vee (K_1 \cup K_{2s-3})$ and $\alpha = \frac{3}{n-1}$, then $s = 2$, which means that $G \cong C_4$, it contradicts with G is an irregular graph.

(6) If $G = K_1 \vee 2K_{\frac{n-1}{2}}$ and $\alpha = \frac{2}{n+1}$, then $n = 1$, it contradicts with $n \geq 3$.

To summarize, both of the graphs listed above don't satisfy the condition. Thus, there is no extremal graph. If $s = 1$, then $Spec_{A_\alpha}(G) = \{\tau + \frac{2\alpha m}{n}, [\frac{2\alpha m}{n}]^{n-1}\}$ by (2.9), which means G has two distinct eigenvalues exactly and $G \cong K_n$, a contradiction. □

3. The conclusion remark

Remark 3.1. *Denote ρ_1 and ρ_n the largest A_α-eigenvalue and the minimum A_α-eigenvalue, separately. Sorting $\gamma_i = |\rho_j - \frac{2\alpha m}{n}|$ and ρ_i $(i, j = 1, \ldots, n)$ in the decreasing order, if $\rho_1 + \rho_n \geq \frac{4\alpha m}{n}$, then $\gamma_i = |\rho_i - \frac{2\alpha m}{n}|$ and ρ_i $(i, j = 1, \ldots, n)$ in the decreasing order. And $\gamma_i = |\rho_i - \frac{2\alpha m}{n}|(i = 1, n)$ occurs if $\rho_1 + \rho_n \geq \frac{4\alpha m}{n}$, there are many graphs satisfying the condition such as $K_{n,n}\backslash F$, $K_{n_1,n_2}(n_1 + n_2 \geq 4)$, K_n, $K_{1,n-1}$ $(n \geq 4)$, C_n(n is even), where F is a perfect matching of $K_{n,n}$.*

In this section, we give some lower and upper bounds of $E^{A_\alpha}(G)$ under the condition that $\rho_1 + \rho_n \geq \frac{4\alpha m}{n}$.

Lemma 3.2. [1] Let $\{d_1, d_2, \ldots, d_n\}$ be the degree sequence of G, then

$$d_1^2 + d_2^2 + \cdots + d_n^2 \leq m(\frac{2m}{n-1} + n - 2),$$

the equality holds if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Lemma 3.3. *Let G be a simple graph with n vertices, m edges and $\alpha \in [0, 1]$, ρ_1 is the A_α-spectral radius of G. Then*

$$\rho_1 \leq \frac{2\alpha m + \sqrt{m[n^3\alpha^2 + n^2(2 - 4\alpha - \alpha^2) + n(4\alpha - 2 - 2\alpha^2 m) + 4\alpha^2 m]}}{n},$$

the equality holds if and only if $G \cong K_n$.

Proof. *By Cauchy-Schwarz inequality, we have*

$$(\rho_2 + \cdots + \rho_n)^2 \leq (n - 1)({\rho_2}^2 + \cdots + {\rho_n}^2).$$

By the above inequalities and equations (2.1) and (2.2) and Lemma 3.2, we have

$$\begin{cases} (\sum_{i=1}^n \rho_i - \rho_1)^2 \leq (n-1)(\sum_{i=1}^n \rho_i^2 - \rho_1^2), \\ (2\alpha m - \rho_1)^2 \leq (n-1)[2(1-\alpha)^2 m + \alpha^2 m(\frac{2m}{n-1} + n - 2) - \rho_1^2]. \end{cases}$$

Thus,

$$n\rho_1^2 - 4\alpha m\rho_1 + 2\alpha^2 m^2 - 2(1-\alpha)^2 m(n-1) - \alpha^2 m(n-1)(n-2) \leq 0.$$

That is

$$\rho_1 \leq \frac{2m\alpha + \sqrt{m[n^3\alpha^2 + n^2(2 - 4\alpha - \alpha^2) + n(4\alpha - 2 - 2\alpha^2 m) + 4\alpha^2 m]}}{n}.$$

Note that $Spec_{A_\alpha}(K_n) = \{n-1, [\alpha n - 1]^{n-1}\}$ and $Spec_{A_\alpha}(K_{1,n}) = \{\frac{n\alpha \pm \sqrt{(n\alpha)^2 + 4(n-1)(1-\alpha)}}{2}, [\alpha]^{n-2}\}$. If $G = K_n$, it is obvious that the equality holds. On the other hand, the equality holds if and only if $\rho_2 = \rho_3 = \cdots = \rho_n$ by the Cauchy-Schwarz inequality. Thus, $G \cong K_n$. □

Lemma 3.4. [14] Let A, x, y and B be some positive real numbers such that $0 < A \leq x \leq y \leq B$. Then $\frac{\sqrt{AB}}{A+B} \leq \frac{\sqrt{xy}}{x+y}$, the equality holds if and only if $x = A$ and $y = B$.

Lemma 3.5. [11] Let G be an undirected connected graph with $n \geq 2$ vertices and m edges. Then $M_1 \geq \frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2$, the equality holds if and only if G is isomorphic with k-regular graph, $1 \leq k \leq n - 1$.

When generalizing $\gamma_n \geq \frac{\sqrt{c}}{2n}$, we simplify of the lower bound in Theorem 1.1 by evaluating $\frac{\sqrt{\gamma_1\gamma_n}}{\gamma_1+\gamma_n}$ and get the extremal graph.

Corollary 3.6. *Let G be a connected graph with $n \geq 2$ vertices and $m \geq 1$ edges, $\alpha \in [\frac{1}{2}, 1)$, if $\gamma_n \geq \frac{\sqrt{c}}{2n}$ and $\alpha \in [\frac{1}{2}, 1)$, where $c = m[n^3\alpha^2 + n^2(2 - 4\alpha - \alpha^2) + n(4\alpha - 2 - 2\alpha^2 m) + 4\alpha^2 m]$, then*

$$E^{A_\alpha}(G) \geq \frac{2\sqrt{2}}{3}\sqrt{[2(1-\alpha)^2 m + \frac{1}{2}\alpha^2(\Delta - \delta)^2]n},$$

if G is regular, the equality holds if and only if $G \cong K_3$.

Proof. We have $\gamma_1 = |\rho_1 - \frac{2\alpha m}{n}| \leq \frac{2\alpha m + \sqrt{m[\alpha^2 n^3 + n^2(2-4\alpha-\alpha^2) + n(4\alpha - 2 - 2\alpha^2 m) + 4\alpha^2 m]}}{n} - \frac{2\alpha m}{n} = \frac{\sqrt{c}}{n}$ by Lemma 3.3. Thus, $\frac{\sqrt{c}}{2n} \leq \gamma_n \leq \gamma_1 \leq \frac{\sqrt{c}}{n}$ and $\frac{\sqrt{\gamma_1\gamma_n}}{\gamma_1 + \gamma_n} \geq \frac{\sqrt{\frac{\sqrt{c}}{2n}\frac{\sqrt{c}}{n}}}{\frac{\sqrt{c}}{2n} + \frac{\sqrt{c}}{n}} = \frac{\sqrt{2}}{3}$ by Lemma 3.4. By Theorem 1.1 and Lemma 3.5, we have

$$\begin{aligned} E^{A_\alpha}(G) &\geq 2\sqrt{[2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}]n} \cdot \frac{\sqrt{\gamma_1\gamma_n}}{\gamma_1 + \gamma_n} \\ &\geq \frac{2\sqrt{2}}{3}\sqrt{[2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}]n} \\ &\geq \frac{2\sqrt{2}}{3}\sqrt{[2(1-\alpha)^2 m + \frac{1}{2}\alpha^2(\Delta - \delta)^2]n}, \end{aligned}$$

if G is regular, then the equality holds if and only if $gK_{\frac{2m}{n}+1} \bigcup h(K_{\frac{2m}{n}+1, \frac{2m}{n}+1} \backslash F)$ or $G \cong \frac{n}{2}K_2$, $\frac{\sqrt{c}}{n} = \gamma_1$, $\frac{\sqrt{c}}{2n} = \gamma_n$ and G is a connected regular graph, where $\frac{2m}{n} \geq 2$ is an integer.

Since G is connected, $G \cong K_{\frac{2m}{n}+1, \frac{2m}{n}+1} \backslash F$ or $G \cong K_{\frac{2m}{n}+1}$, where F is a perfect matching of G, and $2(\frac{2m}{n} + 1) = n$, $m = \frac{n}{2}(\frac{n}{2} - 1)$. Thus, $K_{\frac{2m}{n}+1, \frac{2m}{n}+1} = K_{\frac{n}{2}, \frac{n}{2}}$. Similarly, we have $K_{\frac{2m}{n}+1} = K_n$. If $G \cong K_{\frac{n}{2}, \frac{n}{2}} \backslash F$, then $(1-\alpha)(\frac{n}{2} - 1) = |\rho_1 - \frac{2\alpha m}{n}| = \gamma_1 = \frac{\sqrt{c}}{n} = \frac{\sqrt{\frac{\alpha^2}{8}n^5 + (\frac{1}{2} - \alpha)n^4 - \frac{1}{2}(2\alpha^2 - 6\alpha + 3)n^3 + (1-\alpha)^2 n^2}}{n}$, where $c = m[n^3\alpha^2 + n^2(2 - 4\alpha - \alpha^2) + n(4\alpha - 2 - 2\alpha^2 m) + 4\alpha^2 m]$. We have $n = 2$ or $n = \frac{2(2\alpha - 1)}{\alpha^2}$. If $n = 2$, then $m = 0$. Since $\alpha \in [\frac{1}{2}, 1)$, $n = \frac{2(2\alpha-1)}{\alpha^2} < 2$, a contradiction. If $G \cong K_n$, then $\gamma_1 = \frac{\sqrt{c}}{n} = (n-1)(1-\alpha)$, where $c = [n(n-1)(1-\alpha)]^2$. On the other hand, since $|(\alpha n - 1) - \alpha r| = |\rho_n - \frac{2\alpha m}{n}| = \gamma_n = \frac{\sqrt{c}}{2n} = (1-\alpha)\frac{n-1}{2}$, $n = 3$. Therefore, the equality holds if and only if $G \cong K_3$.

Conversely, note that $Spec_{A_\alpha}(K_3) = \{2, [3\alpha - 1]^2\}$, the equality holds if $n = m = 3$ and $\rho_1 + \rho_n > \frac{4\alpha m}{n}$. □

Lemma 3.7. [12] Let G be a graph with $\Delta(G) = \Delta$, $A(G) = A$, and $A_\alpha(G) = A_\alpha$. Then $\rho(A_\alpha) \leq \alpha\Delta + (1-\alpha)\rho(A)$, the equality holds if and only if G has an r-regular component.

Corollary 3.8. *Let G be a connected graph with n vertices and m edges, $\alpha \in [\frac{1}{2}, 1)$, if $\gamma_n = 0$. Then*

(1) if G is regular, then

$$E^{A_\alpha}(G) \geq (1-\alpha)n,$$

the equality holds if and only if $G \cong K_{\frac{n}{2}, \frac{n}{2}}$.

(2) if G is irregular, then

$$E^{A_\alpha}(G) > \frac{2(1-\alpha)^2 m + \frac{\alpha^2(\Delta-\delta)^2}{2}}{\alpha\Delta + (1-\alpha)\rho(A) - \frac{2\alpha m}{n}}.$$

Proof. We have $\gamma_1 = \rho_1 - \frac{2\alpha m}{n} \leq \alpha\Delta + (1-\alpha)\rho(A) - \frac{2\alpha m}{n}$ by Lemma 3.7. By Theorem 1.2 and Lemma 3.5, then

$$E^{A_\alpha}(G) \geq \frac{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}}{\gamma_1} \geq \frac{2(1-\alpha)^2 m + \frac{\alpha^2(\Delta-\delta)^2}{2}}{\alpha\Delta + (1-\alpha)\rho(A) - \frac{2\alpha m}{n}}.$$

The equality holds if and only if $G \cong K_{\frac{n}{2}, \frac{n}{2}}$ by Lemma 3.7 and G is a regular graph. Note that $\frac{2(1-\alpha)^2 m + \frac{\alpha^2(\Delta-\delta)^2}{2}}{\alpha\Delta + (1-\alpha)\rho(A) - \frac{2\alpha m}{n}} = (1-\alpha)n$ if G is regular, and $G \cong K_{\frac{n}{2}, \frac{n}{2}}$. If G is irregular, then (2) is obvious. □

Note that a regular graph that is neither complete nor empty of order n is called strongly regular with parameters (n, r, a, c) if it is r-regular, every pair of adjacent vertices has a common neighbors and every pair of nonadjacent vertices has c common neighbors. We define $S(n, r)$ is a strongly regular graph whose indices is $(n, r, \frac{r(n-r)}{n-1}, \frac{r(n-r)}{n-1})$.

Theorem 3.9. *Let G be a graph with n vertices and m edges, M_1 be the first Zagreb index, and $\alpha \in [\frac{1}{2}, 1)$. Then*

(1) if $n > \frac{4[(1-\alpha)^2+\alpha^2]m^2}{2m(1-\alpha)^2+\alpha^2 M_1}$, then

$$E^{A_\alpha}(G) \leq \sqrt{\frac{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}}{n}} + \sqrt{(n-1)[2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n} - \frac{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}}{n}]},$$

the equality holds if and only if $G \cong K_2$, $G \cong \frac{n}{2}K_2$ or $G \cong nK_1$.

(2) if $n \leq \frac{4[(1-\alpha)^2+\alpha^2]m^2}{2(1-\alpha)^2 m+\alpha^2 M_1}$, then

$$E^{A_\alpha}(G) \leq \frac{2(1-\alpha)m}{n} + \sqrt{(n-1)\{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n} - [\frac{2(1-\alpha)m}{n}]^2\}},$$

the equality holds if and only if $G \cong K_n$, $G \cong \frac{n}{2}K_2$ or $G \cong S(n, r)$.

Proof. By (2.5) and Cauchy-Schwatz inequality, we have

$$\begin{aligned} E^{A_\alpha}(G) &= \sum_{i=1}^{n} |\gamma_i| \\ &= |\gamma_1| + \sum_{i=2}^{n} |\gamma_i| \\ &\leq \gamma_1 + \sqrt{(n-1)\sum_{i=2}^{n} \gamma_i^2} \\ &= \gamma_1 + \sqrt{(n-1)(\sum_{i=1}^{n} \gamma_i^2 - \gamma_1^2)} \\ &= \gamma_1 + \sqrt{(n-1)[2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n} - \gamma_1^2]}. \end{aligned} \tag{3.1}$$

Set $f(x) = x + \sqrt{(n-1)[2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n} - x^2]}$, where $x \in [0, \sqrt{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}}]$, and $f'(x) = 1 + \sqrt{n-1} \cdot \frac{-x}{\sqrt{2(1-\alpha)^2 m+\alpha^2 M_1 - \frac{4(\alpha m)^2}{n} - x^2}}$. Suppose $f'(x) = 0$, we have $x = \sqrt{\frac{2(1-\alpha)^2 m+\alpha^2 M_1-\frac{4(\alpha m)^2}{n}}{n}}$. Let $U_1 = [0, \sqrt{\frac{2(1-\alpha)^2 m+\alpha^2 M_1-\frac{4(\alpha m)^2}{n}}{n}}]$ and $U_2 = [\sqrt{\frac{2(1-\alpha)^2 m+\alpha^2 M_1-\frac{4(\alpha m)^2}{n}}{n}}, \sqrt{2(1-\alpha)^2 m + \alpha^2 M_1 - \frac{4(\alpha m)^2}{n}}]$. Clearly, $f(x)$ increases on U_1 and decreases on U_2. We have $\gamma_1 = \rho_1 - \frac{2\alpha m}{n} \geq \frac{2(1-\alpha)m}{n}$ by Lemma 2.6, consequently,

$$\begin{cases} f(\gamma_1) \leq f(\sqrt{\frac{2(1-\alpha)^2 m+\alpha^2 M_1-\frac{4(\alpha m)^2}{n}}{n}}), & if\ \frac{2(1-\alpha)m}{n} \in U_1. \\ f(\gamma_1) \leq f(\frac{2(1-\alpha)m}{n}), & if\ \frac{2(1-\alpha)m}{n} \in U_2. \end{cases}$$

Next, we will discuss in the following two situations.

Case 1. $\frac{2(1-\alpha)m}{n} \in U_1$. Then $\frac{2(1-\alpha)m}{n} < \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}}$, and so $n > \frac{4[(1-\alpha)^2+\alpha^2]m^2}{2m(1-\alpha)^2+\alpha^2M_1} > 1$, $(4[(1-\alpha)^2+\alpha^2]m^2 - (2m(1-\alpha)^2+\alpha^2M_1) = (1-\alpha)^2[(d_1+d_2+\cdots+d_n)^2-(d_1+d_2+\cdots+d_n)]+\alpha^2[(d_1+d_2+\cdots+d_n)^2-(d_1^2+d_2^2+\cdots+d_n^2)] > 0)$. Thus, we have

$$\begin{aligned}E^{A_\alpha}(G) &\leq f(\gamma_1)\\ &\leq f(\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}})\\ &= \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}}\\ &+ \sqrt{\frac{(2(1-\alpha)^2m+\alpha^2M_1)(n^2-1)-4(\alpha m)^2(n-\frac{1}{n})}{n}},\end{aligned} \tag{3.2}$$

the equality holds if and only if $\gamma_2 = \gamma_3 = \cdots = \gamma_n$ and $\gamma_1 = \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}}$.

If (3.2) is an equality, then $\gamma_1 = \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}}$ and $\gamma_i = |\rho_i - \frac{2\alpha m}{n}| = \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}-\gamma_1^2}{n-1}} = \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}}$ for $i = 2,3,\ldots,n$. We have $\rho_1 = \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} + \frac{2\alpha m}{n}$ and

$$\{\rho_i(2 \leq i \leq n)\} \subseteq \{\frac{2\alpha m}{n} \pm \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}}\} \tag{3.3}$$

If G is connected, then $Spec_{A_\alpha}(G) = \{\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} + \frac{2\alpha m}{n}, [-\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} + \frac{2\alpha m}{n}]^{n-1}\}$ by (3.3), we have $(2-n)\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} = 0$ by equation (2.1), then $n = 2$ or $\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} = 0$. If $n = 2$, then $G \cong K_2$; If $\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} = 0$, then $Spec_{A_\alpha}(G) = \{[\frac{2\alpha m}{n}]^n\}$, and $G \cong nK_1$, it contradicts with G connected. Thus, $G \cong K_2$. If G is non-connected, then there exists $2 \leq b < n$ such that $Spec_{A_\alpha}(G) = \{[\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} + \frac{2\alpha m}{n}]^{b+1}, [-\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} + \frac{2\alpha m}{n}]^{n-b-1}\}$ by (3.3). Then $(2b+2-n)\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} = 0$ by equation (2.1). If $n = 2b+2$, then $Spec_{A_\alpha}(G) = \{[\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} + \frac{2\alpha m}{n}]^{b+1}, [-\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} + \frac{2\alpha m}{n}]^{b+1}\}$. Similarly, $G \cong \frac{n}{2}K_2$. If $\sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}} = 0$, then $Spec_{A_\alpha}(G) = \{[\frac{2\alpha m}{n}]^n\}$ and $G \cong nK_1$. Thus, $G \cong nK_1$ or $G \cong \frac{n}{2}K_2$.

Case 2. $\frac{2(1-\alpha)m}{n} \in U_2$. Then $\frac{2(1-\alpha)m}{n} \geq \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}}{n}}$, and so $n \leq \frac{4[(1-\alpha)^2+\alpha^2]m^2}{2(1-\alpha)^2m+\alpha^2M_1}$. Thus, we have

$$\begin{aligned}E^{A_\alpha}(G) &\leq f(\gamma_1)\\ &\leq f(\frac{2(1-\alpha)m}{n})\\ &= \frac{2(1-\alpha)m}{n} + \sqrt{(n-1)\{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}-[\frac{2(1-\alpha)m}{n}]^2\}},\end{aligned} \tag{3.4}$$

the equality holds if and only if $\gamma_2 = \gamma_3 = \cdots = \gamma_n$ and $\gamma_1 = \frac{2(1-\alpha)m}{n}$ which means that $\rho_1 = \frac{2m}{n}$. Note that G is an $r = \frac{2m}{n}$ regular graph by Lemma 2.6. If (3.4) is an equality, then G is an $r = \frac{2m}{n}$ regular graph and $\gamma_i = |\rho_i - \frac{2\alpha m}{n}| = \sqrt{\frac{2(1-\alpha)^2m+\alpha^2M_1-\frac{4(\alpha m)^2}{n}-\gamma_1^2}{n-1}} = (1-\alpha)\sqrt{\frac{r(n-r)}{n-1}}$ for $i = 2, 3, \ldots, n$. Thus we have

$$\{\rho_2, \rho_3, \cdots, \rho_n\} \subseteq \{(1-\alpha)\sqrt{\frac{r(n-r)}{n-1}} + \alpha r, (\alpha-1)\sqrt{\frac{r(n-r)}{n-1}} + \alpha r\} \text{ and } \rho_1 = r. \tag{3.5}$$

If G is connected, then A_α-spectra of G has the following three cases:

Subcase 2.1. $Spec_{A_\alpha}(G) = \{r, [(1-\alpha)\sqrt{\frac{r(n-r)}{n-1}}+\alpha r]^{n-1}\}$. Then $\sqrt{\frac{r(n-r)}{n-1}} = \frac{-r}{n-1} < 0$ by equation (2.1), a contradiction.

Subcase 2.2. $Spec_{A_\alpha}(G) = \{r, [(\alpha-1)\sqrt{\frac{r(n-r)}{n-1}}+\alpha r]^{n-1}\}$. Then $\sqrt{\frac{r(n-r)}{n-1}} = \frac{r}{n-1} = n-r$ and $Spec_{A_\alpha}(G) = \{r, [\alpha n-1]^{n-1}\}$, and $G \cong K_n$.

Subcase 2.3. $Spec_{A_\alpha}(G) = \{r, [(1-\alpha)\sqrt{\frac{r(n-r)}{n-1}} + \alpha r]^b, [(\alpha-1)\sqrt{\frac{r(n-r)}{n-1}} + \alpha r]^{n-b-1}\}$. It's obvious that G is strongly regular by Lemma 2.4. Note that for a strongly r-regular graph G, $Spec_{A_0}(G) = \{r, [h]^a, [s]^b\}$ if and only if $Spec_{A_\alpha}(G) = \{r, [\alpha r + (1-\alpha)h]^a, [\alpha r + (1-\alpha)s]^b\}$. Thus, $Spec_{A_0}(G) = \{r, [\sqrt{\frac{r(n-r)}{n-1}}]^b, [(-\sqrt{\frac{r(n-r)}{n-1}}]^{n-b-1}\}$. If G is a strongly regular graph whose indices is (n, r, a, c), $\sqrt{\frac{r(n-r)}{n-1}}$ and $-\sqrt{\frac{r(n-r)}{n-1}}$ as A-eigenvalues of G satisfying the function $x^2 - (a-c)x - (r-c) = 0$ and $r + b\sqrt{\frac{r(n-r)}{n-1}} + (n-b-1)(-\sqrt{\frac{r(n-r)}{n-1}}) = 0$, after simple calculus, then $a = c = \frac{r(r-1)}{n-1}$ and $b = \frac{(n-1)\sqrt{r-c}-r}{2\sqrt{r-c}}$. Consequently, G is a strongly regular graph whose indices is $(n, r, \frac{r(n-r)}{n-1}, \frac{r(n-r)}{n-1})$. Obviously, $G \cong S(n, r)$. If G is non-connected, then there exists $2 \leq b < n$ such that $Spec_{A_\alpha}(G) = \{[r]^{b+1}, [(\alpha-1)\sqrt{\frac{r(n-r)}{n-1}} + \alpha r]^{n-b-1}\}$ and $\sqrt{\frac{r(n-r)}{n-1}} = r = 1$ by (3.5). We have $n = 2b+2$ by equation (2.1), then $Spec_{A_\alpha}(G) = \{[1]^{\frac{n}{2}}, [2\alpha-1]^{\frac{n}{2}}\}$. Thus, $G \cong \frac{n}{2}K_2$. We have accomplished the proof. □

Lemma 3.10. [2] Let G be a connected graph with n vertices and m edges, M_1 is the first Zagreb index of G. Then $M_1 \leq \frac{4m^2}{n} + \frac{n}{4}(\Delta-\delta)^2$, the equality holds if and only if G is isomorphic with k-regular graph.

Nextly, we will simplify the bound given in Theorem 3.9.

Corollary 3.11. *Let G be a connected irregular graph with n vertices and m edges, $\alpha \neq 0$. Then*

(1) if $n > \frac{4(1-\alpha)m\sqrt{(1-\alpha)^2+\alpha^2(\Delta-\delta)^2}-(1-\alpha)}{\alpha^2(\Delta-\delta)^2}$, *then*

$$E^{A_\alpha}(G) < \sqrt{\frac{2(1-\alpha)m^2}{n} + \frac{\alpha^2}{4}(\Delta-\delta)^2} + (n-1)\sqrt{\frac{8m(1-\alpha)^2 + \alpha^2(\Delta-\delta)^2 n}{4n}}.$$

(2) if $n \leq \frac{4(1-\alpha)m\sqrt{(1-\alpha)^2+\alpha^2(\Delta-\delta)^2}-(1-\alpha)}{\alpha^2(\Delta-\delta)^2}$, *then*

$$E^{A_\alpha}(G) < \frac{2(1-\alpha)m}{n} + \sqrt{(n-1)\{2(1-\alpha)^2m + \frac{\alpha^2 n}{4}(\Delta-\delta)^2 + [\frac{2(1-\alpha)m}{n}]^2\}}.$$

Proof. By (3.1) *and Lemma 3.10, we have*

$$E^{A_\alpha}(G) \leq \gamma_1 + \sqrt{(n-1)[2(1-\alpha)^2m + \frac{\alpha^2 n}{4}(\Delta-\delta)^2 - \gamma_1^2]}.$$

The inequality should be strictly if G is a connected irregular graph, then set

$$g(x) = x + \sqrt{(n-1)[2(1-\alpha)^2m + \frac{\alpha^2 n}{4}(\Delta-\delta)^2 - x^2]},$$

where $x \in [0, \sqrt{2(1-\alpha)^2 m + \frac{\alpha^2 n}{4}(\Delta-\delta)^2}]$. *It is similar to the proof of Theorem 3.9,* $g(x)$ *increases on* $I_1 = [0, \sqrt{\frac{2(1-\alpha)^2 m}{n} + \frac{\alpha^2}{4}(\Delta-\delta)^2}]$ *and decreases on* $I_2 = [\sqrt{\frac{2(1-\alpha)^2 m}{n} + \frac{\alpha^2}{4}(\Delta-\delta)^2}, \sqrt{2(1-\alpha)^2 m + \frac{\alpha^2 n}{4}(\Delta-\delta)^2}]$. *Then* $\gamma_1 = \rho_1 - \frac{2\alpha m}{n} > \frac{2(1-\alpha)m}{n}$ *by Lemma 2.6, we have*

$$\begin{cases} E^{A_\alpha}(G) < g(\gamma_1) \le g(\sqrt{\frac{2(1-\alpha)^2 m}{n} + \frac{\alpha^2 n}{4}(\Delta-\delta)^2}), & if\ \frac{2(1-\alpha)m}{n} \in I_1. \\ E^{A_\alpha}(G) < g(\gamma_1) \le g(\frac{2(1-\alpha)m}{n}), & if\ \frac{2(1-\alpha)m}{n} \in I_2. \end{cases}$$

$\frac{2(1-\alpha)m}{n} \in I_1$ *if and only if* $n > \frac{4(1-\alpha)m[\sqrt{(1-\alpha)^2+\alpha^2(\Delta-\delta)^2}-(1-\alpha)]}{\alpha^2(\Delta-\delta)^2}$ *and* $\frac{2(1-\alpha)m}{n} \in I_2$ *if and only if* $n \le \frac{4(1-\alpha)m[\sqrt{(1-\alpha)^2+\alpha^2(\Delta-\delta)^2}-(1-\alpha)]}{\alpha^2(\Delta-\delta)^2}$. □

If G is a regular graph, then $M_1 = nr^2$ and $2m = nr$, we have the upper bound of $E^{A_\alpha}(G)$ of regular graph directly.

Corollary 3.12. *Let G be a connected r-regular graph with order n,* $\alpha \in [0, 1]$. *Then*

(1) if $n > \frac{nr[(1-\alpha)^2+\alpha^2]}{(1-\alpha)^2+\alpha^2 r}$, *then*

$$E^{A_\alpha}(G) \le n\sqrt{r}(1-\alpha)$$

the equality holds if and only if $G \cong K_2$, $G \cong \frac{n}{2}K_2$ *or* $G \cong nK_1$.

(2) if $n \le \frac{nr[(1-\alpha)^2+\alpha^2]}{(1-\alpha)^2+\alpha^2 r}$, *then*

$$E^{A_\alpha}(G) \le (1-\alpha)(r + \sqrt{r(n-r)(n-1)}),$$

the equality holds if and only if $G \cong K_n$, $G \cong \frac{n}{2}K_2$ *or* $G \cong S(n, r)$.

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