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Sharp Upper Bounds for Energy and Randić Energy

Şerife Burcu Bozkurt[1], **Durmuş Bozkurt**

Department of Mathematics, Science Faculty,
Selçuk University, 42075, Campus, Konya, Turkey,
`srf_burcu_bozkurt@hotmail.com` , `dbozkurt@selcuk.edu.tr`

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Abstract

Sharp upper bounds for the energy and Randić energy of a (bipartite) graph are established. From these, some previously known results could be deduced.

1 Introduction

Let G be a graph with n vertices and m edges. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of G. For $1, 2, \ldots, n$ let d_i be the degree (=number of first neighbors) of the vertex v_i. The 2-degree of the vertex v_i [6], denoted by t_i, is the sum of the degrees of the vertices adjacent to v_i. If any two vertices v_i and v_j are adjacent, then we use the notation $v_i \sim v_j$.

Let $A(G) = (a_{ij})$ be the adjacency matrix of the graph G where $a_{ij} = 1$ if $v_i \sim v_j$ and $a_{ij} = 0$ otherwise. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of $A(G)$. These eigenvalues are said to be the eigenvalues of G and to form its spectrum [9]. The largest eigenvalue λ_1 is called the spectral radius of G. Note that if G is a connected graph, then $A(G)$ is an irreducible matrix, then by the Perron Fobenius Theory of non-negative matrices, the spectral radius λ_1 has multiplicity one and there exists a unique positive unit eigenvector corresponding to it [2].

[1]Corresponding author

The Randić matrix $R = R(G) = [R_{ij}]$ of G is the $n \times n$ matrix as the following

$$R_{ij} = \begin{cases} \frac{1}{\sqrt{d_j\, d_j}} & v_i \sim v_j \\ 0 & \text{otherwise.} \end{cases}$$

Randić matrix was studied in connection with the Randić index [1, 23, 24]. It (denoted by A^*, but without any name and without any mention of the Randić index) was found in the seminal book by Cvetković, Doob, and Sachs [9] (p. 26). Also, the role of Randić matrix in the Laplacian spectral theory was clarified in [5]. The Randić eigenvalues of the graph G are the eigenvalues of its Randić matrix and denoted by $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. The largest Randić eigenvalue ρ_1 is called the Randić spectral radius of G. It was proved that Randić spectral radius $\rho_1 = 1$ [9, 20].

Let $L(G) = D(G) - A(G)$ be the Laplacian matrix of the graph G, where $A(G)$ and $D(G)$ are the adjacency matrix and the diagonal matrix of the vertex degrees of G, respectively. The normalized Laplacian matrix [8] of G is defined as

$$\triangle(G) = D(G)^{-1/2} L(G) D(G)^{-1/2}$$

where $D(G)^{-1/2}$ is the matrix obtained by taking the $\left(-\frac{1}{2}\right)$-power of each entry of $D(G)$. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ be the eigenvalues of $\triangle(G)$. These eigenvalues are called the normalized Laplacian eigenvalues of G. For a graph G without isolated vertices, it can be seen that the normalized Laplacian matrix and Randić matrix are related as follows [5]

$$\triangle(G) = I - R(G)$$

where, I is the $n \times n$ unit matrix and $R(G)$ is the Randić matrix.

The energy of the graph G is defined as [10]

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

The concept of graph energy is closely related to total π-electron energy in a molecule represented by a (molecular) graph. An extensive work has been done on graph energy. For details, see [10–12, 15, 17–19, 21, 22, 27, 28].

In line with the general ideas by which the energy concept is extended to the other graph matrices [19], Randić energy pertaining to Randi ć matrix is defined as [5]

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i| \,. \tag{2}$$

Recently, the concept of Randić energy was studied intensely in the literature. For more information, see [3–5, 20, 25].

In view of the fact that the normalized Laplacian eigenvalues of a graph G with no isolated vertices are nonnegative real numbers and their sum is equal to n [8], where n is the number of vertices of G, the normalized Laplacian analogue of Eq. (1), namely the normalized Laplacian energy, is defined as [7]

$$\triangle E = \triangle E(G) = \sum_{i=1}^{n} |\mu_i - 1| \, . \tag{3}$$

For details and some bounds on normalized Laplacian energy, see [7].

This paper is organized in the following way. In Section 2, we give some working lemmas which will be used in our main results. In Section 3, we obtain a lower bound for the spectral radius of a graph. In Section 4, we establish sharp upper bounds for the energy of a (bipartite) graph. From which, we also arrive at some known results. In Section 5, we characterize the upper bound on Randić energy obtained in [20] and present a sharp upper bound for the Randić energy of a bipartite graph.

2 Preliminary Lemmas

Lemma 2.1. [14] *Let A be a nonnegative symmetric matrix and x be a unit vector of $\mathbb{R}^n$. If $\lambda_1(A) = x^T Ax$, then $Ax = \lambda_1(A)\, x$.*

Lemma 2.2. [4] *A simple connected graph G has two distinct Randić eigenvalues if and only if G is complete.*

Lemma 2.3. [5] *If G is a graph without isolated vertices, then the normalized Laplacian energy defined via Eq. (3) coincides with the Randić energy defined via Eq. (2).*

Considering Lemma 2.3, we can give the following lemma.

Lemma 2.4. [7] *Let G be a graph with n vertices and no isolated vertices. Then*

$$RE(G) \geq 2$$

with equality if and only if G is a complete multipartite graph.

3 A lower bound for the spectral radius of a graph

Let $\mathbb{R}^+$ denotes the set of positive real numbers. Let G be a connected graph with n vertices and let $b_i \in \mathbb{R}^+$, $1 \le i \le n$. In order to obtain a lower bound for the spectral radius of G, we define the following sequence

$$S_i^{(1)}, S_i^{(2)}, \ldots, S_i^{(t)}, \ldots$$

where $S_i^{(1)} = b_i$ and $S_i^{(t)} = \sum\limits_{i \sim j} S_j^{(t-1)}$, for each $t \ge 2$, $t \in \mathbb{Z}$.

Theorem 1. *Let G be a connected graph with n vertices and let $b_i \in \mathbb{R}^+$, $1 \le i \le n$. Then*

$$\lambda_1(G) \ge \max_t \max_{b_i} \left\{ \sqrt{\frac{\sum\limits_{i=1}^{n} \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} \right\}. \tag{4}$$

Moreover, the equality holds in (4) for a particular value of t if and only if

$$\frac{S_1^{(t+1)}}{S_1^{(t)}} = \frac{S_2^{(t+1)}}{S_2^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}}$$

or G is a bipartite graph with the partition $\{v_1, v_2, \ldots, v_r\} \cup \{v_{r+1}, \ldots, v_n\}$ and

$$\frac{S_1^{(t+1)}}{S_1^{(t)}} = \cdots = \frac{S_r^{(t+1)}}{S_r^{(t)}} \quad , \quad \frac{S_{r+1}^{(t+1)}}{S_{r+1}^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}} .$$

Proof. Let $X = (x_1, x_2, \ldots, x_n)^T$ be the unit positive Perron eigenvector of $A(G)$ corresponding to λ_1. Now we take the unit positive vector

$$C = \frac{1}{\sqrt{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} \left(S_1^{(t)}, S_2^{(t)}, \ldots, S_n^{(t)}\right)^T.$$

Then we have

$$\lambda_1(G) = \sqrt{\lambda_1\left(A(G)^2\right)} = \sqrt{X^T A(G)^2 X} \ge \sqrt{C^T A(G)^2 C} \,. \tag{5}$$

Since

$$\begin{aligned} AC &= \frac{1}{\sqrt{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} \left(\sum_{j=1}^{n} a_{1j} S_j^{(t)}, \sum_{j=1}^{n} a_{2j} S_j^{(t)}, \ldots, \sum_{j=1}^{n} a_{nj} S_j^{(t)}\right)^T \\ &= \frac{1}{\sqrt{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} \left(S_1^{(t+1)}, S_2^{(t+1)}, \ldots, S_n^{(t+1)}\right)^T \end{aligned}$$

we get

$$\lambda_1(G) \geq \sqrt{C^T A(G)^2 C} = \sqrt{\frac{\sum_{i=1}^{n} \left(S_i^{(t+1)}\right)^2}{\sum_{i=1}^{n} \left(S_i^{(t)}\right)^2}} .$$

Hence the inequality (4) holds. Now we assume that the equality holds in (4). By Eq. (5) and Lemma 2.1, $A(G)^2 C = \lambda_1\left(A(G)^2\right) C$. Then, C is a positive eigenvector of $A(G)^2$ corresponding to $\lambda_1\left(A(G)^2\right)$. If the multiplicity of the eigenvalue $\lambda_1\left(A(G)^2\right)$ is one, then by Perron Frobenius Theorem, C is also an eigenvector of $A(G)$ corresponding to $\lambda_1(G)$. Therefore $A(G)C = \lambda_1(G)C$ which implies $\frac{S_i^{(t+1)}}{S_i^{(t)}} = \lambda_1(G)$, $1 \leq i \leq n$. If the multiplicity of the eigenvalue of $\lambda_1\left(A^2(G)\right)$ is two, then $-\lambda_1\left(A(G)\right)$ is also an eigenvalue of $A(G)$. Then G is a bipartite graph (see, Theorem 3.4. in [9]) and the adjacency matrix $A(G)$ of G can be taken as the following form

$$A(G) = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

where B is an $r \times (n-r)$ matrix. Let

$$X = (X_1, X_2)^T \qquad \text{and} \qquad C = \frac{1}{\sqrt{\sum_{i=1}^{n} \left(S_i^{(t)}\right)^2}} (C_1, C_2)^T$$

where $X_1 = (x_1, \ldots, x_r)^T$, $X_2 = (x_{r+1}, \ldots, x_n)^T$, $C_1 = \left(S_1^{(t)}, \ldots, S_r^{(t)}\right)^T$ and $C_2 = \left(S_{r+1}^{(t)}, \ldots, S_n^{(t)}\right)^T$. Since

$$A(G)^2 = \begin{pmatrix} BB^T & 0 \\ 0 & B^T B \end{pmatrix}$$

we have

$$BB^T C_1 = \lambda_1\left(A(G)^2\right) C_1 \quad , \quad B^T B C_2 = \lambda_1\left(A(G)^2\right) C_2$$

and

$$BB^T X_1 = \lambda_1\left(A(G)^2\right) X_1 \quad , \quad B^T B X_2 = \lambda_1\left(A(G)^2\right) X_2 .$$

Note that BB^T and $B^T B$ are similar matrices. Then $\lambda_1\left(A(G)^2\right)$ is the eigenvalue both of the matrices BB^T and $B^T B$ with multiplicity one. Therefore $X_1 = a_1 C_1$ and $X_2 = a_2 C_2$, that is,

$$\frac{S_1^{(t+1)}}{S_1^{(t)}} = \cdots = \frac{S_r^{(t+1)}}{S_r^{(t)}} \qquad \text{and} \qquad \frac{S_{r+1}^{(t+1)}}{S_{r+1}^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}} .$$

Conversely, considering the similar method in the proof of Theorem 4 in [26] and by some simple calculations, it can be easily seen that the result holds. □

Remark 3.1. From Theorem 1, we have the following results:

i) Taking $b_i = 1$ and $t = 1$ in (4), we have the Hofmeister's bound in [13].

ii) Taking $b_i = d_i$ and $t = 1$ in (4), we have the Yu et al's bound in [26].

iii) Taking $b_i = d_i$ and $t = 2$ in (4), we have the Hong and Zhang's bound in [14].

iv) Taking $b_i = d_i$ and $t = 3$ in (4), we have the Hu's bound in [16].

v) Taking $b_i = d_i$ in (4), we have the Hou et al's bound in [15].

Remark 3.2. Note that the bound (4) is also more general than the Liu and Lu's bound in [22].

4 Energy of a (bipartite) graph

In this section, we obtain sharp upper bounds for the energy of a (bipartite) graph. Note that $S_i^{(1)} = b_i$ and $S_i^{(t)} = \sum\limits_{i\sim j} S_j^{(t-1)}$, for each $t \geq 2$, $t \in \mathbb{Z}$, where $b_i \in \mathbb{R}^+$, $1 \leq i \leq n$.

Theorem 2. *Let G be a connected graph with n vertices and m edges and let t be an integer. Then*

$$E(G) \leq \min_t \min_{b_i} \left\{ \sqrt{\frac{\sum\limits_{i=1}^n \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^n \left(S_i^{(t)}\right)^2}} + \sqrt{(n-1)\left(2m - \frac{\sum\limits_{i=1}^n \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^n \left(S_i^{(t)}\right)^2}\right)} \right\}. \tag{6}$$

Moreover, the equality holds in (6) for a particular value of t if and only if $G \cong K_n$ or G is a non-bipartite connected graph satisfying

$$\frac{S_1^{(t+1)}}{S_1^{(t)}} = \frac{S_2^{(t+1)}}{S_2^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}}$$

and has three distinct eigenvalues

$$\left(p \ , \ \sqrt{\frac{2m-p^2}{n-1}} \ , \ -\sqrt{\frac{2m-p^2}{n-1}}\right)$$

where

$$p = \frac{S_i^{(t+1)}}{S_i^{(t)}} > \sqrt{\frac{2m}{n}} \ , \ 1 \leq i \leq n \ .$$

Proof. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of the graph G. Using Cauchy–Schwarz Inequality, we get

$$E(G) \leq \lambda_1 + \sum_{i=2}^n |\lambda_i| \leq \lambda_1 + \sqrt{(n-1)\sum_{i=2}^n \lambda_i^2} = \lambda_1 + \sqrt{(n-1)\left(2m - \lambda_1^2\right)} \ .$$

By Theorem 1, Remark 3.1, and Theorem 4.1 in [22] , we have

$$\begin{aligned}\lambda_1 &\geq \max_t \max_{b_i} \left\{ \sqrt{\frac{\sum\limits_{i=1}^{n} \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} \right\} \geq \max_t \max_{b_i=d_i} \left\{ \sqrt{\frac{\sum\limits_{i=1}^{n} \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} \right\} \\ &\geq \sqrt{\frac{\left(\sum\limits_{i=1}^{n} t_i\right)^2}{n \sum\limits_{i=1}^{n} d_i^2}} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} d_i^2} \geq \sqrt{\frac{2m}{n}} \, . \qquad (7)\end{aligned}$$

Consider the auxiliary function

$$f(x) = x + \sqrt{(n-1)(2m - x^2)}$$

for $x \leq \sqrt{2m}$ and note that it is monotonically decreasing for $x \geq \sqrt{\frac{2m}{n}}$, see [28]. Therefore, we get

$$E(G) \leq f(\lambda_1) \leq f\left(\sqrt{\frac{\sum\limits_{i=1}^{n} \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} \right) .$$

Hence the inequality (6) holds. If the equality holds in (6), then by similar method in the proof of Theorem 2.5 in [21], we conclude that G is one of the two graphs specified in the second part of the theorem.

Conversely, it can be easily seen that the equality holds in (6) for the graphs specified in the second part of the theorem. □

Considering (7) and the similar procedure in the proof of Theorem 3.1 in [21], we can give the following result.

Theroem 3. *Let G be a connected bipartite graph with $n > 2$ vertices and m edges and let t be an integer. Then*

$$E(G) \leq \min_t \min_{b_i} \left\{ 2\sqrt{\frac{\sum\limits_{i=1}^{n} \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}} + \sqrt{(n-2)\left(2m - \frac{2\sum\limits_{i=1}^{n} \left(S_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n} \left(S_i^{(t)}\right)^2}\right)} \right\} . \qquad (8)$$

Moreover, the equality holds in (8) for a particular value of t if and only if $G \cong K_{r_1,r_2} \cup (n - r_1 - r_2) K_1$, where $r_1 r_2 = m$ or G is a connected bipartite graph with the partitions

$V_1 = \{v_1, v_2, \dots, v_r\}$ $V_2 = \left\{v_{r+1}, \dots, v_n\right\}$, *such that*

$$\frac{S_1^{(t+1)}}{S_1^{(t)}} = \cdots = \frac{S_r^{(t+1)}}{S_r^{(t)}} \quad , \quad \frac{S_{r+1}^{(t+1)}}{S_{r+1}^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}}$$

and has four distinct eigenvalues

$$\left(\sqrt{p_1\, p_2}\ ,\ \sqrt{\frac{2m - 2p_1\, p_2}{n-2}}\ ,\ -\sqrt{\frac{2m - 2p_1\, p_2}{n-2}}\ ,\ -\sqrt{p_1\, p_2}\right)$$

where

$$\begin{aligned} p_1 &= \frac{S_i^{(t+1)}}{S_i^{(t)}}\ ,\ 1 \le i \le r \\ p_2 &= \frac{S_j^{(t+1)}}{S_j^{(t)}}\ ,\ r+1 \le j \le n \end{aligned}$$

$$\sqrt{p_1\, p_2} > \sqrt{\frac{2m}{n}}\ .$$

Remark 4.1. From Theorem 2 and Theorem 3, we have the following results:

i) i) Taking $b_i = 1$ and $t = 1$ in (6) and (8), we have the Zhou's bounds in [28].

ii) Taking $b_i = d_i$ and $t = 1$ in (6) and (8), we have the Yu et al's bounds in [27].

iii) Taking $b_i = d_i$ and $t = 2$ in (6) and (8), we have the Liu et al's bounds in [21].

iv) Taking $b_i = d_i$ in (6) and (8), we have the Hou et al's bounds in [15].

Remark 4.2. Note that the bounds (6) and (8) are also more generalized forms of the Liu and Lu's bounds in [22].

5 Randić energy of a (bipartite) graph

In this section, we present our results on Randić energy.

Theoreom 4. *Let G be a connected graph with n vertices. Then*

$$RE(G) \le 1 + \sqrt{(n-1)\left(2\sum_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 1\right)}. \tag{9}$$

Moreover, the equality holds in (9) if and only if G is a complete graph or a non-bipartite connected graph with three distinct Randić eigenvalues

$$\left(1\ ,\ \sqrt{\frac{2\sum\limits_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 1}{n-1}}\ ,\ -\sqrt{\frac{2\sum\limits_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 1}{n-1}}\right). \tag{10}$$

Proof. Inequality (9) was earlier reported in [20]. Now we assume that the equality holds in (9). Then we have

$$\rho_1 = 1 \qquad \text{and} \qquad |\rho_i| = \sqrt{\frac{2\sum\limits_{v_i \sim v_j} \frac{1}{d_i\, d_j} - 1}{n-1}}\ , \quad \text{for } 2 \le i \le n\ .$$

Then there are two possibilities:

• G has exactly two distinct Randić eigenvalues. Then by Lemma 2.2, $G \cong K_n$ for some $n \ge 2$.

• G has exactly three distinct Randić eigenvalues. Since $\rho_1 > \rho_i$ and $\rho_i \ne 0$, for $2 \le i \le n$, we conclude that G is a non-bipartite connected graph with three distinct Randić eigenvalues given by (10).

Conversely, we can easily see that the equality holds in (9) for the graphs specified in the second part of the theorem. □

Now we consider the bipartite graph case of the above theorem.

Theoreom 5. *Let G be a connected bipartite graph with $n \ge 2$ vertices. Then*

$$RE(G) \le 2 + \sqrt{(n-2)\left(2\sum_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 2\right)}\ . \tag{11}$$

Moreover, the equality holds in (11) if and only if G is a complete bipartite graph or a non-complete bipartite graph with four distinct Randić eigenvalues

$$\left(1\ ,\ \sqrt{\frac{2\sum\limits_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 2}{n-2}}\ ,\ -\sqrt{\frac{2\sum\limits_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 2}{n-2}}\ ,\ -1\right). \tag{12}$$

Proof. Let $\rho_1 \ge \rho_2 \ge \cdots \ge \rho_n$ be the Randić eigenvalues of G. Note that

$$\sum_{i=1}^{n} |\rho_i| = RE(G) \qquad \text{and} \qquad \sum_{i=1}^{n} \rho_i^2 = 2\sum_{v_i \sim v_j} \frac{1}{d_j\, d_j}$$

see [5]. Since G is a bipartite graph, we have $\rho_1 = -\rho_n$ [9] (p. 109). Using Cauchy–Schwarz Inequality, we get

$$\sum_{i=2}^{n-1} |\rho_i| \le \sqrt{(n-2)\sum_{i=2}^{n-1} \rho_i^2} = \sqrt{(n-2)\left(2\sum_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 2\rho_1^2\right)}.$$

Therefore

$$RE(G) \leq 2\rho_1 + \sqrt{(n-2)\left(2\sum_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 2\rho_1^2\right)}\ . \tag{13}$$

Combining (13) and $\rho_1 = 1$ [9, 20], we get the inequality (11). Now we suppose that the equality holds in (11). Therefore we have

$$\rho_1 = -\rho_n = 1 \qquad \text{and} \qquad |\rho_i| = \sqrt{\frac{2\sum\limits_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 2}{n-2}} \quad \text{for} \ \ 2 \leq i \leq n-1\ .$$

Then we have the three possibilities.

• G has exactly two distinct Randić eigenvalues. Then, by Lemma 2.2, we conclude that G is a complete bipartite graph of order two.

• G has exactly three distinct Randić eigenvalues. In this case, $\rho_1 = -\rho_n = 1$ and $|\rho_i| = \sqrt{\frac{2}{n-2}\sum\limits_{v_i \sim v_j} \frac{1}{d_j\, d_j} - 2} = 0$, for $2 \leq i \leq n-1$ which implies that $RE(G) = 2\rho_1 = 2$. Then by Lemma 2.4, we conclude that G is a complete bipartite graph.

• G has exactly four distinct Randić eigenvalues. Note that the multiplicity of $\rho_1 = 1$ is one and $\rho_i \neq 0$ for $2 \leq i \leq n-1$. Then G is non-complete bipartite graph with four distinct Randić eigenvalues given by (12).

Conversely, it can be easily seen that the equality holds in (11) for the graphs specified in the second part of the theorem. $\square$

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