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New Upper Bounds on the Energy of a Graph

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Abstract

The energy of a graph G, denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of all eigenvalues of G. It is proved in [MATCH Commun. Math. Comput. Chem. 79 (2018) 287–301] by Alawiah et al. that $\mathcal{E}(G) \leq 2\sqrt{\Delta} + \sqrt{(n-2)(2m-2\Delta)}$ for every bipartite graph G of order n, size m and maximum degree Δ. We prove the above bound for all graphs G. We also prove new types of two bounds of Koolen and Moulton given in [Adv. Appl. Math. 26 (2001) 47-52] and [Graphs Comb. 19 (2003) 131–135].

1 Introduction

For graph theory notation and terminology not given here we refer to [4]. Let $G = (V, E)$ be a simple undirected graph with vertex set $V = V(G) =$

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$\{v_1, v_2, \ldots, v_n\}$ and edge set E. The *order* and *size* of G are $n = |V|$ and $m = |E|$, respectively. For a vertex $v_i \in V$, the *degree* of v_i, denoted by $\deg(v_i)$, is the number of edges incident with v_i. We denote by $\Delta(G)$ the maximum degree among the vertices of G. A graph G is r-regular if every vertex has degree r. An r-regular graph G is called *strongly regular* if there are integers λ and μ such that every two adjacent vertices have λ common neighbor and every two non-adjacent vertices have μ common neighbors, (see [6]). We denote by $K_{1,n-1}$ a star of order n and by K_n a complete graph of order n. The *adjacency matrix* $A(G)$ of a graph G is defined by its entries as $a_{ij} = 1$ if $v_iv_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ denote the eigenvalues of $A(G)$. When more than one graph are under consideration, we write $\lambda_i(G)$ instead of λ_i. The *second Zagreb index* of a graph G is defined by $M_2(G) = \sum_{uv \in E} d_u d_v$ in [12], and is vastly studied, see for example, [5, 17].

The *incidence matrix* of a 2-(ν, k, λ)-design with ν points $x_1, ..., x_\nu$ and b blocks $B_1, ..., B_b$ is the $\nu \times b$ matrix $B = (b_{ij})$, where $b_{ij} = 1$ if $x_i \in B_j$ and 0 otherwise. The *incidence graph* of a design is defined to be the graph with adjacency matrix

$$\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}.$$

It is known that the incidence graph of a symmetric 2-(ν, k, λ)-desig with $\nu > k > \lambda > 0$ has eigenvalues k, $\sqrt{k-\lambda}$ (with multiplicity $\nu - 1$), $-\sqrt{k-\lambda}$ (with multiplicity $\nu - 1$), and $-k$, (See [8], 10.3).

The graph energy is an invariant that was defined by Gutman [11] in his studies of mathematical chemistry. The *energy* of a graph G is defined as

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

This concept is now a well studied concept, (see, for example, [1], [9]-[16], [18]). Many researchers presented bounds for the energy of a graph. Recently, Alawiah et al. [2] proved the following for bipartite graphs.

Theorem 1 ([2]). *Let G be a non-empty bipartite graph with $n \geqslant 2$*

vertices, m edges and maximum vertex degrees Δ. Then

$$\mathcal{E}(G) \leq 2\sqrt{\Delta} + \sqrt{(n-2)(2m-2\Delta)},$$

equality holds if and only if $G \cong \frac{n}{2}K_2$ *or* $K_{1,\Delta} \bigcup (n-\Delta-1)K_1$.

Koolen and Moulton [14] and [15] proved the following.

Theorem 2 ([14]). *If $2m \geqslant n$ and G is a graph with n vertices, m edges, then*

$$\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left(2m - (\frac{2m}{n})^2\right)}.$$

Equality holds if and only if G is either $\frac{n}{2}K_2$, K_n, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{n-1}}$.

Theorem 3 ([15]). *If $2m \geqslant n$ and G is a bipartite graph with $n \geq 2$ vertices, m edges, then*

$$\mathcal{E}(G) \leq 2\left(\frac{2m}{n}\right) + \sqrt{(n-2)\left(2m - 2(\frac{2m}{n})^2\right)}.$$

Equality holds if and only if $G = \frac{n}{2}K_2$, $K_{\sqrt{m},\sqrt{m}}$, where $n = 2\sqrt{m}$, or G is the incidence graph of a symmetric 2-(ν, k, λ) design, where $\nu = \frac{n}{2}$, $k = \frac{2m}{n}$, $\lambda = \frac{k(k-1)}{n-1}$ and $2\sqrt{m} < n < 2m$.

In this paper, we extend Theorem 1 by proving its validity for all graphs. We also prove new types of Theorems 2 and 3. In Section 3, we prove an upper bound for the energy of a graph in terms of order, size and the maximum degree of the graph. In Section 3, we prove two upper bounds for the energy of a graph in terms of order, size and the second Zagreb index.

2 Useful lemmas and theorems

The following results play important roles in the proof of our main results.

Theorem 4 ([3]). *If $A = (a_{ij})$ is a Hermitian matrix with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$, then*

$$|\lambda_1 - \lambda_n|^2 \geq \max_{i,j}\{(a_{ii} - a_{jj})^2 + 2\sum_{k\neq i}|a_{ik}|^2 + 2\sum_{k\neq j}|a_{jk}|^2\}.$$

Theorem 5 ([4], Corollary 5.6). *If G is a connected graph and H is a proper induced subgraph of G, then $\lambda_1(H) < \lambda_1(G)$.*

Lemma 1 ([7]). *If G is a non-empty graph of order $n \geqslant 2$ and size m, and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G, then $\lambda_1 + |\lambda_i| \leq 2\sqrt{m}$ for $2 \leq i \leq n$.*

Lemma 2 ([17]). *If G is a graph with n vertices and m edges, then $\frac{M_2}{m} \geqslant \frac{4m^2}{n^2}$.*

Lemma 3 ([6]). *If a connected graph G has m distinct eigenvalues, then its diameter D satisfies the inequality $D \leq m - 1$.*

Theorem 6 ([6]). *A regular connected graph G is strongly regular if and only if it has exactly three distinct eigenvalues.*

3 An upper bound involving maximum degree

We first need to prove the following lemma.

Lemma 4. *If G is a non-empty graph of order $n \geqslant 2$ with maximum degree Δ, and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G, then $\lambda_1 + |\lambda_n| \geq 2\sqrt{\Delta}$.*

Proof. Let A be the adjacency matrix of G and denote $\deg(v_i) = \Delta$. By Theorem 4,

$$|\lambda_1 - \lambda_n|^2 \geq (a_{ii} - a_{ii})^2 + 2\sum_{k\neq i}|a_{ik}|^2 + 2\sum_{k\neq i}|a_{ik}|^2 = 4\Delta.$$

Thus, $\lambda_1 + |\lambda_n| = |\lambda_1 - \lambda_n| \geq 2\sqrt{\Delta}$, as desired. ■

Now, we prove the main result of this section.

Theorem 7. *Let G be a non-empty graph with $n \geqslant 2$ vertices, m edges and maximum vertex degrees Δ. Then*

$$\mathcal{E}(G) \leq 2\sqrt{\Delta} + \sqrt{(n-2)(2m-2\Delta)},$$

equality holds if and only if $G \cong \frac{n}{2}K_2$ or $G \cong K_{1,\Delta}\bigcup(n-\Delta-1)K_1$.

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of G. Using the Cauchy-Schwartz inequality,

$$\begin{aligned}
\mathcal{E}(G) &= \sum_{j=1}^{n}|\lambda_j| = \lambda_1 + |\lambda_n| + \sum_{j=2}^{n-1}|\lambda_j| && (1)\\
&\leq \lambda_1 + |\lambda_n| + \sqrt{(n-2)(2m-\lambda_1^2-\lambda_n^2)} && (2)\\
&= \lambda_1 + |\lambda_n| + \sqrt{(n-2)(2m+2\lambda_1|\lambda_n|-(\lambda_1+|\lambda_n|)^2)} && (3)\\
&\leq \lambda_1 + |\lambda_n| + \sqrt{(n-2)(2m-\frac{(\lambda_1+|\lambda_n|)^2}{2})}, && (4)
\end{aligned}$$

since

$$2\lambda_1|\lambda_n| \leq \frac{(\lambda_1+|\lambda_n|)^2}{2}. \tag{5}$$

Let $f(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$. Then f is decreasing for $\sqrt{\frac{2m}{n}} \leq x \leq \sqrt{m}$. By Lemmas 1 and 4,

$$\sqrt{\frac{2m}{n}} \leq \sqrt{\Delta} \leq \frac{\lambda_1+|\lambda_n|}{2} \leq \sqrt{m}. \tag{6}$$

Thus,

$$\mathcal{E}(G) \leq f(\frac{\lambda_1+|\lambda_n|}{2}) \leq f(\sqrt{\Delta}) = 2\sqrt{\Delta} + \sqrt{(n-2)(2m-2\Delta)}. \tag{7}$$

We next prove the equality part. First it is easy to see that equality holds if $G \cong \frac{n}{2}K_2$ or $K_{1,\Delta}\bigcup(n-\Delta-1)K_1$. Thus we prove the converse. Assume that $\mathcal{E}(G) = 2\sqrt{\Delta} + \sqrt{(n-2)(2m-2\Delta)}$. Following the proof of the first part, all inequalities in (2)-(5), the second inequality in (6) and both inequalities in (7) become equalities. From (5) and (6) we obtain that $\lambda_1 = |\lambda_n| = \sqrt{\Delta}$ and from (2), (4) and (7) we obtain that $|\lambda_i| = |\lambda_j| = \sqrt{\frac{2m-2\Delta}{n-2}}$ for all $i, j \in \{2, ..., n-1\}$ and $i \neq j$, if $n > 2$. From $\lambda_1 = |\lambda_n| = \sqrt{\Delta}$, we have $\lambda_n \neq 0$, since G is a non-empty graph. Thus, clearly $\lambda_n < 0$. By the Perron–Frobenius theorem G contains a bipartite component H whose eigenvalues contain λ_1 and λ_n, since $\lambda_1 = -\lambda_n > 0$. Since $K_{1,\Delta}$ is an induced subgraph of G, and $\lambda_1(K_{1,\Delta}) = \sqrt{\Delta}$, by Theorem 5, we may assume that $H = K_{1,\Delta}$. If $\Delta > 1$, then H has eigenvalue 0, and we deduce that $|\lambda_j| = 0$ for all $j \in \{2, ..., n-1\}$. Hence each other component of G is a K_1. Consequently, $G = K_{1,\Delta} \bigcup (n - \Delta - 1)K_1$. Thus assume that $\Delta = 1$. Then $\lambda_1 = 1$ and each component of G is a K_2 or K_1. If $m = 1$, then $G = K_{1,\Delta} \bigcup (n - \Delta - 1)K_1$. Thus assume that $m > 1$. Then $|\lambda_j| = \sqrt{\frac{2m-2\Delta}{n-2}} \neq 0$ for each $j \in \{2, ..., n-1\}$. Consequently, $G \cong \frac{n}{2}K_2$. ■

4 Upper bounds involving the second Zagreb index

In this section we prove two upper bounds for the energy of a graph in terms of order, size and the second Zagreb index.

Theorem 8. *If $2m \geqslant n$ and G is a graph of order n and size m, then*

$$\mathcal{E}(G) \leq \sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-1)\left(2m - \sqrt[3]{(\frac{2M_2}{n})^2}\right)},$$

and equality holds if and only if G is $\frac{n}{2}K_2$, K_n or a non-complete connected strongly regular graph of degree k with eigenvalues k, $\sqrt{\frac{k(n-k)}{n-1}}$ and $-\sqrt{\frac{k(n-k)}{n-1}}$.

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of G. Using the Cauchy-Schwartz inequality,

$$\mathcal{E}(G) \;=\; \sum_{j=1}^{n} |\lambda_j| = \lambda_1 + \sum_{j=2}^{n} |\lambda_j| \leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}.$$

Let $g(x) = x + \sqrt{(n-1)(2m - x^2)}$. Then g is decreasing for $\sqrt{\frac{2m}{n}} \leq x \leq \sqrt{2m}$. Clearly $\lambda_1 \leq \sqrt{2m}$. By Lemma 2 we can easily see that $\sqrt{\frac{2m}{n}} \leq \sqrt[3]{\frac{2M_2}{n}}$. It is evident that

$$2M_2 = (d_1\ d_2\ \ldots\ d_n)A(d_1\ d_2\ \ldots\ d_n)^T = j^T A^3 j,$$

where j is an n by 1 vector whose all components is 1. Now by the Rayleigh's inequality,

$$\frac{2M_2}{n} = \frac{j^T A^3 j}{j^T j} \leq \lambda_1^3. \tag{8}$$

Thus,

$$\sqrt{\frac{2m}{n}} \leq \sqrt[3]{\frac{2M_2}{n}} \leq \lambda_1 \leq \sqrt{2m}. \tag{9}$$

Then $\mathcal{E}(G) \leq g(\lambda_1) \leq g(\sqrt[3]{\frac{2M_2}{n}}) = \sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-1)\Big(2m - \sqrt[3]{(\frac{2M_2}{n})^2}\Big)}$, as desired.

We next prove the equality part. If $G = \frac{n}{2}K_2$ then $\mathcal{E}(G) = n$ and $m = M_2 = \frac{n}{2}$ and thus the equality holds. If $G = K_n$, then $\mathcal{E}(G) = 2(n-1)$, $m = \frac{n(n-1)}{2}$ and $M_2 = \frac{n(n-1)^3}{2}$, and so the equality holds. Now, assume that G is a non-complete connected strongly regular graph of degree k with eigenvalues k, $\sqrt{\frac{k(n-k)}{n-1}}$ and $-\sqrt{\frac{k(n-k)}{n-1}}$. It can be seen that $M_2 = \frac{nk^3}{2}$. Clearly, $\lambda_1 = k = \frac{2m}{n}$. By Theorem 2,

$$\begin{aligned}\mathcal{E}(G) &= \frac{2m}{n} + \sqrt{(n-1)\Big(2m - (\frac{2m}{n})^2\Big)} = k + \sqrt{(n-1)(2m-k^2)} \\ &= \sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-1)\Big(2m - \sqrt[3]{(\frac{2M_2}{n})^2}\Big)}.\end{aligned}$$

For the converse assume that

$$\mathcal{E}(G) = \sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-1)\Big(2m - \sqrt[3]{(\frac{2M_2}{n})^2}\Big)}.$$

Following the proof, we obtain that $\lambda_1 = \sqrt[3]{\frac{2M_2}{n}}$ and $|\lambda_j| = \sqrt{\frac{2m - \sqrt[3]{(\frac{2M_2}{n})^2}}{(n-1)}}$ for $j = 2, ..., n$. From $\lambda_1 = \sqrt[3]{\frac{2M_2}{n}}$, we have $\lambda_1 \neq 0$, since G is a non-empty graph. If $\lambda_1 = |\lambda_j|$ for all $j = 2, ..., n$, then G has exactly two disctinct eigenvalues and so by Lemma 3 each component of G is a complete graph. Since $\lambda_1 = |\lambda_n|$ we deduce that $G = \frac{n}{2}K_2$. We next assume that $\lambda_1 \neq |\lambda_j|$ for all $j = 2, ..., n$. If $\lambda_j = \lambda_{j'}$ for all $j, j' = 2, ..., n$, then by Lemma 3, G is a complete graph. Thus assume that G has exactly three distinct eigenvalues.

By (8) we find that $\frac{j^T A^3 j}{j^T j} = \lambda_1^3$. Let α be an eigenvector corresponding to λ_1 for A. Then $A^3\alpha = \lambda_1^3\alpha$. Since the multiplicity of λ_1^3 for A^3 is 1, by the Perron-Frobenius Theorem $\alpha = cj$ for some c, that is, $Aj = \lambda_1 j$. Consequently, G is a regular graph. By Theorem 6, G is strongly regular, and the proof is complete. ■

Theorem 9. *If $2m \geqslant n$ and G is a bipartite graph with $n \geq 2$ vertices, m edges, then*

$$\mathcal{E}(G) \leq 2\sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-2)\left(2m - 2(\sqrt[3]{\frac{2M_2}{n}})^2\right)}.$$

Equality holds if and only if $G = \frac{n}{2}K_2$, $K_{\sqrt{m},\sqrt{m}}$, where $n = 2\sqrt{m}$, or G is the incidence graph of a symmetric 2-(ν, $\sqrt[3]{\frac{2M_2}{n}}$, λ) design, where $\nu = \frac{n}{2}$, $k = \sqrt[3]{\frac{2M_2}{n}}$ and $\lambda = \frac{k(k-1)}{n-1}$.

Proof. We follow the proof of Theorem 7. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of G. Using the Cauchy-Schwartz inequality,

$$\begin{aligned}\mathcal{E}(G) &= \sum_{j=1}^{n} |\lambda_j| = \lambda_1 + |\lambda_n| + \sum_{j=2}^{n-1} |\lambda_j| \\ &\leq \lambda_1 + |\lambda_n| + \sqrt{(n-2)(2m - \lambda_1^2 - \lambda_n^2)} \\ &\leq \lambda_1 + |\lambda_n| + \sqrt{(n-2)(2m - \frac{(\lambda_1 + |\lambda_n|)^2}{2})}.\end{aligned}$$

The function $f(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$ is decreasing for $\sqrt{\frac{2m}{n}} \leq$

$x \le \sqrt{m}$. Since $\lambda_1^2+\lambda_n^2+\sum_{i=2}^{n-1}\lambda_i^2 = 2m$ and $\lambda_1 = |\lambda_n|$, we have $\lambda_1 \le \sqrt{m}$ and from (8) we obtain that,

$$\sqrt{\frac{2m}{n}} \le \sqrt[3]{\frac{2M_2}{n}} \le \frac{\lambda_1+|\lambda_n|}{2} \le \sqrt{m}. \tag{10}$$

Thus,

$$\begin{aligned}\mathcal{E}(G) \le f(\frac{\lambda_1+|\lambda_n|}{2}) &\le f(\sqrt[3]{\frac{2M_2}{n}}) \\ &= 2\sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-2)\Big(2m-2(\sqrt[3]{\frac{2M_2}{n}})^2\Big)}.\end{aligned}$$

We next prove the equality part. First it is easy to see that equality holds if $G = \frac{n}{2}K_2$, $K_{\sqrt{m},\sqrt{m}}$, where $n = 2\sqrt{m}$. If G is the incidence graph of a symmetric 2-(ν, k, λ) design, where $k = \sqrt[3]{\frac{2M_2}{n}}$ and $\lambda = \frac{k(k-1)}{n-1}$, then by [14] (Page 132), we can see that

$$\mathcal{E}(G) = 2k + (2\nu-2)\sqrt{k-\lambda} = 2\sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-2)\Big(2m-2(\sqrt[3]{\frac{2M_2}{n}})^2\Big)}.$$

Now, we prove the converse. Assume that

$$\mathcal{E}(G) = 2\sqrt[3]{\frac{2M_2}{n}} + \sqrt{(n-2)\Big(2m-2(\sqrt[3]{\frac{2M_2}{n}})^2\Big)}.$$

Then $\lambda_1 = |\lambda_n| = \sqrt[3]{\frac{2M_2}{n}}$ and $|\lambda_j| = \sqrt{\frac{2m-2(\sqrt[3]{\frac{2M_2}{n}})^2}{n-2}}$ for all $j = 2, ..., n-1$, if $n > 2$. The result is obvious if $n = 2$. Assume that $n > 2$. If G has exactly two distinct eigenvalues then by Lemma 3, $G = \frac{n}{2}K_2$. If G has three distinct eigenvalues, then $|\lambda_j| = \sqrt{\frac{2m-2(\sqrt[3]{\frac{2M_2}{n}})^2}{n-2}} = 0$ for all $j = 2, ..., n-1$, and so we obtain that $\lambda_1 = \sqrt{m}$ and $M_2 = \frac{mn\sqrt{m}}{2}$. Since G has three distinct eigenvalues, using Lemma 3 we find that G is a complete bipartite graph. Let X and Y be the partite sets of G, where $|X| = x$ and $|Y| = y$. Clearly, $n = x + y$ and $m = xy$. Since $M_2 = (xy)^2 = \frac{mn\sqrt{m}}{2}$, we obtain that $n = 2\sqrt{m}$. Consequently, $G = K_{\sqrt{m},\sqrt{m}}$. It remains to assume that G has four distinct eigenvalues. Since, $\sqrt[3]{\frac{2M_2}{n}} > \sqrt{\frac{2m-2(\sqrt[3]{\frac{2M_2}{n}})^2}{n-2}}$, by [6] (Page 166), G is the incidence graph of a symmetric 2-(ν, $\sqrt[3]{\frac{2M_2}{n}}$, λ) design, where $\nu = \frac{n}{2}$, $k = \sqrt[3]{\frac{2M_2}{n}}$ and $\lambda = \frac{k(k-1)}{n-1}$. ■

5 Concluding remarks

We note that by Lemma 2 and the inequality chain (9), we can see that

$$\sqrt{\frac{2m}{n}} \leq \frac{2m}{n} \leq \sqrt[3]{\frac{2M_2}{n}} \leq \lambda_1 \leq \sqrt{2m}. \tag{11}$$

Now the decreasing property of the function g implies that the bound of Theorem 8 is better than the bound of Theorem 2. Furthermore, the bound of Theorem 9 is better than the bound of Theorem 3. Also, in [2] the following bound is presented for any graph G,

$$\mathcal{E}(G) \leq \frac{\sqrt{M_2}}{m} + \sqrt{(n-1)(2m - \frac{M_2}{m^2})} \tag{12}$$

and the following bound is presented for any bipartite graph G,

$$\mathcal{E}(G) \leq 2\frac{\sqrt{M_2}}{m} + \sqrt{(n-2)\left(2m - \frac{2M_2}{m^2}\right)}\,. \tag{13}$$

It is known that $\frac{\sqrt{M_2}}{m} \leq \lambda_1$ (see [7]). Thus by Lemma 2 and inequality chains (10) and (11) we find that $\sqrt{\frac{2m}{n}} \leq \frac{2m}{n} \leq \sqrt[3]{\frac{2M_2}{n}} \leq \frac{\sqrt{M_2}}{m} \leq \lambda_1 \leq \sqrt{2m}$ and $\sqrt{\frac{2m}{n}} \leq \frac{2m}{n} \leq \sqrt[3]{\frac{2M_2}{n}} \leq \frac{\sqrt{M_2}}{m} \leq \lambda_1 \leq \sqrt{m}$ if G is bipartite. Now, the decreasing property of the functions f and g in the proofs of Theorems 8 and 9, implies that the bound of Theorem 8 is better than the bound given in (12) and the bound of Theorem 9 is better than the bound given in (13).

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