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Some sharp lower bounds for energy of graphs

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Abstract: The energy $\mathcal{E}(G)$ of a graph G is the sum of the absolute values of all the eigenvalues of the adjacency matrix of G. It is used in chemistry to approximate the total π-electron energy of a molecule. This paper presented some new lower bounds for $\mathcal{E}(G)$, and characterized those graphs for which these bounds were attained.

Key words: graph; energy; lower bound; interlace; quotient matrix

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图的能量的几个可达下界

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摘要: 图 G 的能量 $\mathcal{E}(G)$ 定义为它的邻接矩阵的所有特征值的绝对值之和, 在化学中, 它用来近似分子的 π 电子总能量. 本文给出了关于图的能量 $\mathcal{E}(G)$ 的几个下界, 同时刻画了达到这些下界的极图.

关键词: 图; 能量; 下界; 插值; 商矩阵

0 Introduction

Let G be a simple graph on n vertices and m edges with vertex set $V(G)$ and edge set $E(G)$. Let $A(G)$ be the adjacency matrix of G. Since $A(G)$ is symmetric, its eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$ are all real, and we assume that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. It is obvious that $\sum_{i=1}^{n} \lambda_i = 0$ according to the zero trace of $A(G)$.

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The *energy* of G, denoted by $\mathcal{E}(G)$, was first defined by Gutman in 1978 as

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

This concept of graph energy arose in chemistry where certain numerical quantities, such as the heat of formation of a hydrocarbon, are related to the total π-electron energy that can be calculated as the energy of an appropriate "molecular" graph(see, e.g., [1-3]). It turns out that the graph energy is not affected by isolated vertices, and the energy of a complete bipartite graph K_{n_1,n_2} is $\mathcal{E}(K_{n_1,n_2})=2\sqrt{n_1n_2}$.

In this work, we are primarily interested in the lower bounds for graph energy. A general lower bound was obtained by McClelland[4] as

$$\mathcal{E}(G)\geqslant\sqrt{2m+n(n-1)|\det A(G)|^{2/n}}. \tag{0.1}$$

A lower bound only in terms of the number of edges is[5]

$$\mathcal{E}(G)\geqslant 2\sqrt{m}. \tag{0.2}$$

And a lower bound depending only on the number of vertices is[5]

$$\mathcal{E}(G)\geqslant 2\sqrt{n-1}. \tag{0.3}$$

This bound (0.3) applies to graphs without isolated vertices, and it can be improved as $\mathcal{E}(G)\geqslant n$ when $\det A(G)\neq 0$ from (0.1)(see [1]). More lower bounds can be found in [1].

In this work, we present some new lower bounds(see Theorems A-B and its consequences Corollaries 2.1-2.4) and also characterize the situation when these bounds are attained. All the proofs will be given in Section 2.

Theorem A Let G be a graph without isolated vertices, which has n vertices and m edges. Suppose G contains two induced subgraphs G_1 and G_2, where G_i has n_i vertices and m_i edges $(i=1,2)$, $V(G_1)\cap V(G_2)=\phi$ and $n_1+n_2=n$.

(1) If $m>m_1+m_2+2\sqrt{m_1m_2}$, then

$$\mathcal{E}(G)\geqslant 2\sqrt{(\frac{m_1}{n_1}-\frac{m_2}{n_2})^2+\frac{(m-m_1-m_2)^2}{n_1n_2}},$$

and equality holds if and only if $G=K_{n_1,n_2}$ and $G_i=n_iK_1$ $(i=1,2)$.

(2) If $m\leqslant m_1+m_2+2\sqrt{m_1m_2}$, then $\mathcal{E}(G)>\dfrac{2m_1}{n_1}+\dfrac{2m_2}{n_2}$.

Theorem B Let G be a k-regular graph with n vertices. Suppose G contains two induced subgraphs G_1 and G_2, where G_i has n_i vertices and m_i edges $(i=1,2)$, $V(G_1)\cap V(G_2)=\phi$ and $n_1+n_2=n$. Then

$$\mathcal{E}(G)\geqslant k+\left|\frac{2m_1}{n_1}+\frac{2m_2}{n_2}-k\right|,$$

and equality holds if and only if $G=K_{k,k}$ and $G_1=G_2=kK_1$.

1 Preliminaries

In this section, we cite some concepts from [6] and give some preliminary results, which will be used in the proofs of our main results about the lower bounds for energy of graphs.

Let $s_1 = (\xi_1, \xi_2, \cdots, \xi_n)$ and $s_2 = (\eta_1, \eta_2, \cdots, \eta_m)$ with $m < n$ be two real tuples in nonincreasing order ($\xi_1 \geqslant \xi_2 \geqslant \cdots \geqslant \xi_n$ and $\eta_1 \geqslant \eta_2 \geqslant \cdots \geqslant \eta_m$). s_2 is said to *interlace* s_1 if

$$\xi_i \geqslant \eta_i \geqslant \xi_{n-m+i} \quad \text{for } i = 1, 2, \cdots, m.$$

Without loss of generality, we assume throughout that all the tuples are real and arranged in nonincreasing order.

Lemma 1.1 Let $s_1 = (\xi_1, \xi_2, \cdots, \xi_n)$ and $s_2 = (\eta_1, \eta_2, \cdots, \eta_m)$ be two tuples. If s_2 interlace s_1, then

$$\sum_{i=1}^{n} |\xi_i| \geqslant \sum_{i=1}^{m} |\eta_i|,$$

and equality holds if and only if

$$\eta_i = \begin{cases} \xi_i, & 1 \leqslant i \leqslant k, \\ \xi_{n-m+i}, & k+1 \leqslant i \leqslant m, \end{cases} \quad \text{and} \quad \xi_i = 0 \quad \text{for } k+1 \leqslant i \leqslant n-m+k, \tag{1.1}$$

where $k = \big|\{i \,|\, \eta_i \geqslant 0\}\big| \, \big(0 \leqslant k \leqslant m\big)$.

Proof Since $k = \big|\{i \,|\, \eta_i \geqslant 0\}\big|$, we have

$$\xi_i \geqslant \eta_i \geqslant 0 \, (1 \leqslant i \leqslant k) \quad \text{and} \quad 0 > \eta_i \geqslant \xi_{n-m+i} \, (k+1 \leqslant i \leqslant m).$$

Hence,

$$\sum_{i=1}^{n} |\xi_i| \geqslant \sum_{i=1}^{k} |\xi_i| + \sum_{i=n-m+k+1}^{n} |\xi_i| \geqslant \sum_{i=1}^{k} |\eta_i| + \sum_{i=k+1}^{m} |\eta_i| = \sum_{i=1}^{m} |\eta_i|.$$

And it's easy to see that the equality holds if and only if (1.1) holds.

For an induced subgraph G' of a graph G, as is well-known, the eigenvalues of $A(G')$ interlace those of $A(G)$ by using the famous Cauchy's interlacing theorem[7]Theorem 4.3.15. So, as an extra result of this paper, the following corollary immediately follows from Lemma 1.1.

Corollary 1.2[8] Let G' be an induced subgraph of a graph G. Then $\mathcal{E}(G') \leqslant \mathcal{E}(G)$, and the equality holds if and only if $E(G') = E(G)$.

Lemma 1.3 Let $s_1 = (\xi_1, \xi_2, \cdots, \xi_n)$ and $s_2 = (\eta_1, \eta_2)$ be two tuples. Suppose s_2 interlace s_1 and $\sum_{i=1}^{n} \xi_i = 0$. Then $\sum_{i=1}^{n} |\xi_i| = |\eta_1| + |\eta_2|$ if and only if $\xi_1 = -\xi_n = \eta_1 = -\eta_2$ and $\xi_i = 0 \, (i \neq 1, n)$.

Proof The sufficiency part is obvious. For the necessity part, put $k = \big|\{i \,|\, \eta_i \geqslant 0\}\big|$. Then according to the tightness of the inequality in Lemma 1.1, we have

$$\eta_i = \begin{cases} \xi_i, & 1 \leqslant i \leqslant k, \\ \xi_{n-2+i}, & k+1 \leqslant i \leqslant 2, \end{cases} \quad \text{and} \quad \xi_i = 0 \quad \text{for } k+1 \leqslant i \leqslant n-2+k. \tag{1.2}$$

We can claim that $k \neq 0$. Suppose not, i.e., $k = 0$. Then $0 > \eta_1 = \xi_{n-1} \geqslant \eta_2 = \xi_n$ and $\xi_i = 0$ $(i \neq n-1, n)$, which leads to a contradiction because

$$0 < |\eta_1| + |\eta_2| = -\eta_1 - \eta_2 = -\xi_{n-1} - \xi_n = -\sum_{i=1}^{n} \xi_i = 0.$$

Hence, we distinguish between the following two cases.

Case 1 k=1. From (1.2) we have $\eta_1 = \xi_1$, $\eta_2 = \xi_n$ and $\xi_i = 0$ $(i \neq 1, n)$. Since $\sum_{i=1}^{n} \xi_i = 0$, it follows that $\xi_1 = -\xi_n = \eta_1 = -\eta_2$. Therefore, the conclusion is true.

Case 2 k=2. Then $\eta_1 = \xi_1 \geqslant \eta_2 = \xi_2 \geqslant 0$ and $\xi_i = 0$ $(i \neq 1, 2)$. So we have

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

which implies that $\xi_1 = \xi_2 = \cdots = \xi_n = 0$, and thus $\eta_1 = \eta_2 = 0$. Consequently, the conclusion is also true.

Lemma 1.4[9]Theorem 6.5 Let G be a bipartite graph with eigenvalues $\lambda_1 > \lambda_2 > \lambda_3$ with respective multiplicities m_1, m_2 and m_3. Then $\lambda_3 = -\lambda_1$, $\lambda_2 = 0$, $m_3 = m_1$, and G is the direct sum of m_1 complete bipartite graphs K_{r_i,s_i} where $r_i s_i = \lambda_1^2$ $(i = 1, \cdots, m_1)$, and $m_2 - \sum_{i=1}^{m_1}(r_i + s_i - 2)$ isolated vertices.

Lemma 1.5[9]Theorem 6.6 *A* regular graph G has eigenvalues k, 0, and λ_3 if and only if the complement of G is the direct sum of $-\dfrac{k}{\lambda_3} + 1$ complete graphs of order $-\lambda_3$.

Now we cite another important concept from [6]. Let $\boldsymbol{M}$ be a real symmetric block-partitioned matrix. The *quotient matrix* of M is the matrix whose entries are the average row sums of the blocks of M. For example, let $\{1, 2, \cdots, n\}$ be partitioned as $X_1 \cup X_2 \cup \cdots \cup X_m$ with $|X_i| = n_i > 0$. Consider the corresponding blocking

$$\boldsymbol{M}_{n\times n} = \begin{bmatrix} \boldsymbol{M}_{11} & \cdots & \boldsymbol{M}_{1m} \\ \vdots & & \vdots \\ \boldsymbol{M}_{m1} & \cdots & \boldsymbol{M}_{mm} \end{bmatrix},$$

so that $\boldsymbol{M}_{ij}$ is an $n_i \times n_j$ block. Let s_{ij} be the sum of the entries in $\boldsymbol{M}_{ij}$, then the quotient matrix of $\boldsymbol{M}$ is

$$\boldsymbol{Q}_{m\times m} = \begin{bmatrix} \dfrac{s_{11}}{n_1} & \cdots & \dfrac{s_{1m}}{n_1} \\ \vdots & & \vdots \\ \dfrac{s_{m1}}{n_m} & \cdots & \dfrac{s_{mm}}{n_m} \end{bmatrix}.$$

Lemma 1.6[6] Let $\boldsymbol{M}$ be a real symmetric block-partitioned matrix, and $\boldsymbol{Q}$ be the quotient matrix of $\boldsymbol{M}$. Then the eigenvalues of $\boldsymbol{Q}$ interlace the eigenvalues of $\boldsymbol{M}$.

2 Proofs

Proof of Theorem A Due to G_1 and G_2, $A(G)$ has a quotient matrix as

$$\boldsymbol{Q}=\begin{bmatrix}\frac{2m_1}{n_1} & \frac{m-m_1-m_2}{n_1}\\ \frac{m-m_1-m_2}{n_2} & \frac{2m_2}{n_2}\end{bmatrix}$$

with eigenvalues $\mu_1\geqslant\mu_2$. The characteristic polynomial of $\boldsymbol{Q}$ is

$$|xI-\boldsymbol{Q}|=x^2-(\frac{2m_1}{n_1}+\frac{2m_2}{n_2})x+\frac{4m_1m_2-(m-m_1-m_2)^2}{n_1n_2},$$

with $\mu_1+\mu_2=\frac{2m_1}{n_1}+\frac{2m_2}{n_2}\geqslant 0$ and $\mu_1\mu_2=\frac{4m_1m_2-(m-m_1-m_2)^2}{n_1n_2}$.

(1) if $m>m_1+m_2+2\sqrt{m_1m_2}$, then $4m_1m_2<(m-m_1-m_2)^2$. Thus $\mu_1\mu_2<0$ and

$$(|\mu_1|+|\mu_2|)^2=(\mu_1-\mu_2)^2=(\mu_1+\mu_2)^2-4\mu_1\mu_2=4\big((\frac{m_1}{n_1}-\frac{m_2}{n_2})^2+\frac{(m-m_1-m_2)^2}{n_1n_2}\big).$$

Using Lemma 1.6 and 1.1, we have

$$\mathcal{E}(G)=\sum_{i=1}^{n}|\lambda_i|\geqslant|\mu_1|+|\mu_2|=2\sqrt{(\frac{m_1}{n_1}-\frac{m_2}{n_2})^2+\frac{(m-m_1-m_2)^2}{n_1n_2}}. \tag{2.1}$$

Now if $G=K_{n_1,n_2}$, then $\mathcal{E}(G)=2\sqrt{n_1n_2}$. With $G_i=n_iK_1$ $(i=1,2)$, we have $m_1=m_2=0$ and $m=n_1n_2$, it's easy to verify that the equality holds.

Conversely, if the equality in (2.1) holds, by Lemma 1.3, we have $\lambda_1=-\lambda_n=\mu_1=-\mu_2$ and $\lambda_i=0$ $(i\neq 1,n)$. Since $0=\mu_1+\mu_2=\frac{2m_1}{n_1}+\frac{2m_2}{n_2}$, it follows that $m_1=m_2=0$, i.e., $G_i=n_iK_1$ $(i=1,2)$. So G is a bipartite graph. Moreover, from Lemma 1.4 we deduce that $G=K_{r,s}\cup(n-r-s)K_1$, where $rs=\lambda_1^2=-\mu_1\mu_2=\frac{m^2}{n_1n_2}=\frac{(rs)^2}{n_1n_2}$, i.e., $rs=n_1n_2$. Since G has no isolated vertices, we have $r+s=n(=n_1+n_2)$. And therefore, $G=K_{n_1,n_2}$.

(2) if $m\leqslant m_1+m_2+2\sqrt{m_1m_2}$, then $4m_1m_2\geqslant(m-m_1-m_2)^2$. Thus $\mu_1\mu_2\geqslant 0$. Recall that $\mu_1+\mu_2\geqslant 0$ and we have $\mu_1\geqslant\mu_2\geqslant 0$. Consequently,

$$\mathcal{E}(G)=\sum_{i=1}^{n}|\lambda_i|\geqslant|\mu_1|+|\mu_2|=\mu_1+\mu_2=\frac{2m_1}{n_1}+\frac{2m_2}{n_2}. \tag{2.2}$$

In the following, we will show that the inequality of (2.2) is strict. Suppose to the contrary that the equality in (2.2) holds. According to the proof of Lemma 1.3, we have $\lambda_1=\lambda_2=\cdots=\lambda_n=0$. This implies that G consists of n isolated vertices, which yields a contradiction.

Let G_1 and G_2 be two vertex disjoint graphs, then the *join* of G_1,G_2, denoted by $G_1\vee G_2$, is obtained from their union by including all edges between the vertices in G_1 and the vertices in G_2. A subset S of $V(G)$ is called an *independent set* of G if no two vertices in S are adjacent.

The following Corollary 2.1 and 2.2 are consequences of Theorem A.

Corollary 2.1　Let $G = G_1 \vee G_2$, where each G_i is a graph with n_i vertices and m_i edges $(i = 1, 2)$. Then

$$\mathcal{E}(G) \geqslant 2\sqrt{(\frac{m_1}{n_1} - \frac{m_2}{n_2})^2 + n_1 n_2},$$

and equality holds if and only if $G_i = n_i K_1$ $(i = 1, 2)$.

Proof　Since $m_i \leqslant \dfrac{n_i(n_i - 1)}{2} < \dfrac{n_i^2}{2}$ $(i = 1, 2)$, it follows that $m = m_1 + m_2 + n_1 n_2 > m_1 + m_2 + 2\sqrt{m_1 m_2}$. Then Theorem A gives the result.

Corollary 2.2　Let G be a graph without isolated vertices, which has n vertices and m edges. Suppose S is an independent set of G with $|S| = t$ and $G - S$ having m' edges. Then

$$\mathcal{E}(G) \geqslant 2\sqrt{(\frac{m'}{n - t})^2 + \frac{(m - m')^2}{t(n - t)}},$$

and equality holds if and only if $G = K_{t,n-t}$ and $G - S = (n - t)K_1$.

Proof　Now $n_1 = t, n_2 = n - t, m_1 = 0$ and $m_2 = m'$. It follows that $m > m' = m_1 + m_2 + 2\sqrt{m_1 m_2}$. Then Theorem A gives the result.

Proof of Theorem B　G_1 and G_2 give rise to a partition of $A(G)$ with quotient matrix

$$\boldsymbol{Q} = \begin{bmatrix} \dfrac{2m_1}{n_1} & k - \dfrac{2m_1}{n_1} \\ k - \dfrac{2m_2}{n_2} & \dfrac{2m_2}{n_2} \end{bmatrix}$$

with eigenvalues $\mu_1 = k$ (row sum) and $\mu_2 = \mathrm{tr}(\boldsymbol{Q}) - \mu_1 = \dfrac{2m_1}{n_1} + \dfrac{2m_2}{n_2} - k$. Hence

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i| \geqslant |\mu_1| + |\mu_2| = k + \Big|\frac{2m_1}{n_1} + \frac{2m_2}{n_2} - k\Big|.$$

By Lemma 1.3, the equality holds if and only if $\lambda_1 = -\lambda_n = \mu_1 = -\mu_2 (= k)$ and $\lambda_i = 0$ $(i \neq 1, n)$. And this is true if and only if $\dfrac{2m_1}{n_1} + \dfrac{2m_2}{n_2} - k = -k$ and $G = K_{k,k}$ because of Lemma 1.5, i.e., $m_1 = m_2 = 0$ $(G_1 = G_2 = kK_1)$ and $G = K_{k,k}$.

The following Corollary 2.3 and 2.4 are consequences of Theorem B.

Corollary 2.3　Let G be a k-regular graph with n vertices. Suppose G contains t $(t \geqslant 1)$ independent vertices. Then

$$\mathcal{E}(G) \geqslant \frac{kn}{n - t},$$

and equality holds if and only if $G = K_{k,k}$ and $t = k$.

Proof　Now $n_1 = t, n_2 = n - t, m_1 = 0$ and $m_2 = \dfrac{kn}{2} - kt$. Theorem B gives the result.

Corollary 2.4　Let G be a k-regular graph with n vertices. Suppose G contains an induced subgraph G' with n' $(0 < n' < n)$ vertices and m' edges. Then

$$\mathcal{E}(G) \geqslant k + \Big|\frac{2m'}{n'} - \frac{n'k - 2m'}{n - n'}\Big|,$$

and equality holds if and only if $G = K_{k,k}$ and $G' = kK_1$.

(下转第 38 页)