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New 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] that $\mathcal{E}(G) \leq 2+\sqrt{(n-1)(2m-4)}$ if G is a connected unicyclic graph. We prove a generalization of the above bound for all graphs G. We then prove a new sharp upper bound for the energy of bipartite graphs, and in particular we improve the famous bound $\mathcal{E}(G) \leq \frac{n}{\sqrt{8}}(\sqrt{n}+\sqrt{2})$ of Koolen and Moulton on bipartite graphs given in [Graphs Combin. 19 (2003), 131–135] under certain conditions. We also prove upper and lower bounds for the energy of graphs arisen by the Mycielski construction.

1 Introduction

Let $G = (V, E)$ be a simple undirected graph with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, $\mid E(G) \mid= m$. The *order* and *size* of G are $n = |V|$ and $m = |E|$, respectively. For a vertex $v_i \in V$, the *degree*

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of v_i, denoted by $\deg(v_i)$ (or just d_i), is the number of edges incident to v. We denote by $K_{1,n-1}$ an star of order n and by K_n a complete graph of order n. A *unicyclic* graph is a graph with precisely one cyclic. A *cactus* graph is a graph that any two cycles of G have at most one common vertex. 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 $A(G)$. Then λ_1 is called the *spectral radius* of G. For a graph G Mycielski's construction produces a graph $M(G)$ with $V(M(G)) = V \cup U \cup \{w\}$ where $V = V(G) = \{v_1, ..., v_n\}$, $U = \{u_1, ..., u_n\}$ and $E(M(G)) = E(G) \cup \{u_iv : v \in N_G(v_i) \cup \{w\}, i = 1, ..., n\}$. We define the k-th Mycielski graph of G, recursively by $M^0(G) = G$ and $M^{k+1}(G) = M(M^k(G))$ for $k \geq 1$.

The graph energy is an invariant that was defined by Gutman [8] in his studies of mathematical chemistry. The *energy* of a graph G is defined as

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

This concept is now a well studied concept, ([4, 7, 9, 10, 12, 13]). Many researchers presented bounds for the energy of a graph. Recently, Alawiah et al. [2] proved the following upper bound for the energy of unicyclic graphs.

Theorem 1 ([2]). *Let G be a non-empty, connected unicyclic graph with n vertices and m edges. Then*

$$\mathcal{E}(G) \leq 2 + \sqrt{(n-1)(2m-4)}, \tag{1}$$

equality holds if and only if $G \cong C_3$.

Koolen and Moulton [6] proved the following upper bound for the energy of a bipartite graph.

Theorem 2 ([6]). *Let G be a bipartite graph on $n > 2$ vertices. Then*

$$\mathcal{E}(G) \leq \frac{n}{\sqrt{8}} \left(\sqrt{n} + \sqrt{2}\right).$$

We prove a generalizations of Theorem 1 for all graphs. The generalization is for any graph of order n having size $n-1+k$ for each $k \geq 1$. We then prove a new sharp upper bound for the energy of bipartite graphs that improves Theorem 2 for bipartite graphs of order n and size at least n under certain conditions. We also prove upper and lower bounds for the energy of graphs arisen by the Mycielski construction.

We use the following known results.

Theorem 3 ([1]). *(i) If H_1, ...,H_k is an edge partition of G, then $\mathcal{E}(G) \leq \sum_{i=1}^{k} \mathcal{E}(H_i)$.*
(ii) If H_1, ...,H_k is a vertex partition of G, then $\mathcal{E}(G) \geq \sum_{i=1}^{k} \mathcal{E}(H_i)$.

Theorem 4 ([3]). *If G is a graph with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$, then $\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_i}$.*

Theorem 5 ([11]). *If G is a connected unicyclic graph, then $\lambda_1 \geq 2$.*

2 A new bound on general graphs

In view of Theorem 1, clearly $m = n = (n-1)+1$ for a uncyclic graph G of order n and size m. We thus deduce a new type of Theorem 1 by replacing m with n to read that if G is a non-empty connected unicyclic graph with n vertices, then

$$\mathcal{E}(G) \leq 2 + \sqrt{(n-1)(2n-4)}\,, \tag{2}$$

with equality if and only if $G \cong C_3$. In the following we generalize this for any graph G.

Theorem 6. *If G is a non-empty connected graph of order n and size $m = (n-1)+k$, where $k \geq 1$, then*

$$\mathcal{E}(G) \leq 2k + \sqrt{(n-1)(2n+2k-6)}\,, \tag{3}$$

with equality if and only if $G \cong C_3$.

Proof. We use an induction on k. The base step for $k = 1$ holds by Theorem 1. Thus assume that $k > 1$. Assume the result holds for all connected graphs of order n and size $m' = (n-1)+k'$, where $1 \leq k' < k$. Now consider the graph G of order n and size $m = (n-1)+k$. Observe that G has at least two cycles, since $m = n-1+k \geq n+1$. Let e be an edge of a cycle of G. Let $G' = G - e$. Then G' has size $m' = (n-1)+k'$, where $k' = k-1$. By Theorem 3 (i),

$$\begin{aligned}
\mathcal{E}(G) &\leq 2 + \mathcal{E}(G') \leq 2 + 2k' + \sqrt{(n-1)(2n+2k'-6)} && (4)\\
&= 2k + \sqrt{(n-1)(2n+2k-8)} && (5)\\
&< 2k + \sqrt{(n-1)(2n+2k-6)}\,, && (6)
\end{aligned}$$

as desired. For the equality part, following the above proof, from (6), we find that $k = 1$. Now the result follows from Theorem 1. ■

3 A new bound on bipartite graphs

In this section, we prove a new sharp upper bound for the energy of bipartite graphs.

Theorem 7. *If G is a bipartite graph of order n and size $m = n-1+k$, where $k \geq 1$, then*

$$\mathcal{E}(G) \leq 2k + 2 + \sqrt{(n-2)(2m-2k-6)}\ .$$

This bound is sharp for a cycle C_4.

Proof. The proof is by an induction on the number k. For the basis of the induction, assume that $k = 1$, that is, G is a unicyclic bipartite graph. Let $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$ be the eigenvalues of G. Then $\lambda_n = -\lambda_1$, since G is bipartite. By the Cauchy-Schwartz inequality,

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

It is evident that the function $f(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$ is decreasing for $\sqrt{\frac{2m}{n}} \leq x \leq \sqrt{m}$. Since $\sum_{i=1}^{n} \lambda_i^2 = 2m$, we find that $\lambda_1 \leq \sqrt{m}$. Note that clearly, $n \leq 2m$. Thus by Theorem 5, we find that $\sqrt{\frac{2m}{n}} \leq 2 \leq \lambda_1 \leq \sqrt{m}$. Now,

$$\mathcal{E}(G) \leq f(\lambda_1) \leq f(2) = 4 + \sqrt{(n-2)(2m-8)}\ .$$

Thus the base step of the induction holds. Assume that $k > 1$ and the result is valid for all biprtite graphs of order n and size $m = n - 1 + k'$, where $1 \leq k' < k$. Now consider the bipartite graph G of order n and size $m = n - 1 + k$. Observe that G has at least two cycles, since $m = n - 1 + k \geq n + 1$. Let G' be a bipartite graph arisen from G by removal of an edge e of a cycle of G. Then G' has the same order n and size $m' = m - 1 = n - 1 + k'$, where $k' = k - 1$. Applying the inductive hypothesis, by Theorem 3,

$$\begin{aligned} \mathcal{E}(G) &\leq 2 + \left(2k' + 2 + \sqrt{(n-2)(2m' - 2k' - 6)}\right) \\ &= 2k + 2 + \sqrt{(n-2)(2m - 2k - 6)}\ . \end{aligned}$$

as desired.

To see the sharpness of this bound, consider a cycle C_4, where $n = m = 4$ and $k = 1$, and note that $\mathcal{E}(C_4) = 4$ and $2k+2+\sqrt{(n-2)(2m-2k-6)} = 4$. ■

Corollary 1. *If G is a bipartite graph of order n and size $m = n - 1 + k$, where $k \geq 1$, then*

$$\mathcal{E}(G) \quad \leq \quad 2k + 2 + \sqrt{(n-2)(2n-8)}\ .$$

This bound is sharp.

Comparing the bound of Corollary 1 with the bound of Theorem 2, it is evident that for a wide range of graphs the bound of Corollary 1 is better than the bound of Theorem 2. More precisely, if $k \leq \frac{n}{2\sqrt{8}}(\sqrt{n} + \sqrt{2}) - \frac{1}{2}(\sqrt{(n-2)(2n-8)} - 2)$, then the bound of Corollary 1 is better than the bound of Theorem 2. It is evident that $\frac{n}{2\sqrt{8}}(\sqrt{n} + \sqrt{2}) - \frac{1}{2}(\sqrt{(n-2)(2n-8)} - 2) \to \infty$ as $n \to \infty$, thus we have a wider range of

ks as the order of graph increases. In particular, this happens for graphs with very few edges.

4 Bounds for the energy of Mycielski graphs

We begin with the following observation

Observation 1. *If G is a graph of order n, size m, then*

$$\mathcal{E}(M(G)) \leq \sqrt{n} + \sqrt{2mn + n^2} + \sqrt{4mn}.$$

Proof. Let G be a graph of order n, size m, and $V(G) = \{v_1, ..., v_n\}$. By Theorem 4 and the Cauchy-Schwartz inequality we have

$$\begin{aligned}
\mathcal{E}(M(G)) &\leq \sum_{v \in V(M(G))} \sqrt{\deg_{M(G)}(v)} \\
&= \sqrt{\deg_{M(G)}(w)} + \sum_{i=1}^{n} \sqrt{\deg_{M(G)}(u_i)} + \sum_{i=1}^{n} \sqrt{\deg_{M(G)}(v_i)} \\
&= \sqrt{n} + \sum_{i=1}^{n} \sqrt{d_i + 1} + \sum_{i=1}^{n} \sqrt{2d_i} \\
&\leq \sqrt{n} + \sqrt{n \sum_{i=1}^{n} (d_i + 1)} + \sqrt{n \sum_{i=1}^{n} 2d_i} \\
&= \sqrt{n} + \sqrt{2mn + n^2} + \sqrt{4mn}.
\end{aligned}$$

■

We next prove upper and lower bounds for the energy of $M(G)$ in terms of the energy of G.

Theorem 8. *Let G be a graph of order n, size m, and degree sequence $d_1 \geq d_2 \geq ... \geq d_n$. Then*

$$\mathcal{E}(G) + 2\sqrt{n} \leq \mathcal{E}(M(G)) \leq \mathcal{E}(G) + \min\left\{2\sqrt{n} + 2\sum_{i=1}^{n} \sqrt{d_i}, 2\sum_{i=1}^{n} \sqrt{d_i + 1}\right\}.$$

Proof. We first prove the upper bound. We partition the edge set of $M(G)$ into $n + 2$ partitions as follows. Let $K_{1,n}$ be a star centered at w, and for each vertex $v_i \in V(G)$ let $K_{1,\deg_G(v_i)}$ be a star centered at u_i and its leaves are $N_G(v_i)$. By Theorem 3 (i),

$$\mathcal{E}(M(G)) \leq \mathcal{E}(G) + \mathcal{E}(K_{1,n}) + \sum_{i=1}^{n} \mathcal{E}(K_{1,\deg_G(v_i)}).$$

Noting that $\mathcal{E}(K_{1,n}) = 2\sqrt{n}$ and $\mathcal{E}(K_{1,\deg_G(v_i)}) = 2\sqrt{\deg_G(v_i)}$, we find that $\mathcal{E}(M(G)) \leq \mathcal{E}(G) + 2\sqrt{n} + 2\sum_{i=1}^{n}\sqrt{d_i}$. We next partition the edge set of $M(G)$ into $n+1$ partitions as follows. For each vertex $v_i \in V(G)$ let $K_{1,\deg_G(v_i)+1}$ be a star centered at u_i and its leaves are $N_G(v_i) \cup \{w\}$. By Theorem 3 (i),

$$\mathcal{E}(M(G)) \leq \mathcal{E}(G) + \sum_{i=1}^{n} \mathcal{E}(K_{1,\deg_G(v_i)+1}).$$

Noting that $\mathcal{E}(K_{1,\deg_G(v_i)}) = 2\sqrt{\deg_G(v_i)+1}$, we find that $\mathcal{E}(M(G)) \leq \mathcal{E}(G) + 2\sum_{i=1}^{n}\sqrt{d_i+1}$. Thus the upper bound follows.

We next prove the lower bound. We partition the vertex set of G into two partitions $V(G)$ and $V(M(G)) - V(G)$. Note that the subgraph induced by $V(M(G)) - V(G)$ is $K_{1,n}$. By Theorem 3 (ii), $\mathcal{E}(M(G)) \geq \mathcal{E}(G) + \mathcal{E}(K_{1,n})$. Now the result follows, since $\mathcal{E}(K_{1,n}) = 2\sqrt{n}$. ■

We note that both upper and lower bounds given in Theorem 8 can be achieved, for example if G is an edgeless graph.

Corollary 2. *Let G be a graph of order n, size m, and degree sequence $d_1 \geq d_2 \geq ... \geq d_n$. Then*

(*i*) $\mathcal{E}(M(G)) \leq 2\sqrt{n} + 3\sum_{i=1}^{n}\sqrt{d_i}.$

(*ii*) $\mathcal{E}(M(G)) \leq \sqrt{2n}(\sqrt{2} + 3\sqrt{m}).$

(*iii*) $\mathcal{E}(M(G)) \leq \mathcal{E}(G) + 2\sqrt{n} + 2\sqrt{2mn}.$

(*iv*) $\mathcal{E}(M(G)) \leq \sqrt{\frac{n(M(G))-1}{2}}\left(2 + \sqrt{3}\sqrt{2m(M(G)) - n(M(G)) + 1}\right).$

(*v*) $\mathcal{E}(M(G)) \leq \mathcal{E}(G) + 2\sqrt{n(2m+n)}.$

Proof. (i) This is an immediate consequence of Theorem 4.

(ii) By (i) and the Cauchy-Schwartz inequality we obtain that

$$\mathcal{E}(M(G)) \leq 2\sqrt{n} + 3\sum_{i=1}^{n}\sqrt{d_i} \leq 2\sqrt{n} + 3\sqrt{n\sum_{i=1}^{n} d_i} = 2\sqrt{n} + 3\sqrt{n(2m)}.$$

(iii) This follows by Theorem 8 and the Cauchy-Schwartz inequality.
(iv) This follows from (ii) and the facts that $n(M(G)) = 2n(G) + 1$ and $m(M(G)) = n(G) + 3(m(G))$.
(v) By the Cauchy-Schwartz inequality we obtain that

$$2\sum_{i=1}^{n}\sqrt{d_i + 1} \leq 2\sqrt{n\sum_{i=1}^{n}(d_i + 1)} = 2\sqrt{n(2m + n)}.$$

Now the result follows from Theorem 8. ■

A simple graph G of order n is called *hyperenergetic* if $\mathcal{E}(G) > 2(n-1)$. Balakrishnan [5] showed that if G is a hyperenergetic regular graph of order n with $\mathcal{E}(G) > 3n$, then $M(G)$ is hyperenergetic. It can be seen from the lower bound given in the Theorem 8 that if G is a hyperenergetic graph of order n with $\mathcal{E}(G) > 4n - 2\sqrt{n} + 1$, then $M(G)$ is hyperenergetic.

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