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ORIGINAL PAPER

On the spectral radius of graphs with connectivity at most *k*

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Abstract In this paper, we study the spectral radius of graphs of order n with $\kappa(G) \leq k$. We show that among those graphs, the maximal spectral radius is obtained uniquely at K_n^k, which is the graph obtained by joining k edges from k vertices of K_{n-1} to an isolated vertex. We also show that the spectral radius of K_n^k will be very close to $n-2$ for a fixed k and a sufficiently large n.

Keywords Energy levels · Spectral radius · Connectivity · Edge-connectivity

1 Introduction

In quantum chemistry, the skeletons of certain non-saturated hydrocarbons are represented by graphs. By Hückel molecular orbital (HMO) theory, energy levels of electrons in such a molecule are, in fact, the eigenvalues of the corresponding graph [15]. The stability of the molecule as well as other chemically relevant facts are closely connected with the graph eigenvalues (see [4,9] and [16, Chapters 5 and 6]). In particular, Lovász and Pelikán [14], and Cvetković and Gutman [5] proposed that the spectral radius of the molecular graph (of a saturated hydrocarbon) is used as a measure of branching of the underlying molecule. This direction of research was eventually further elaborated with emphasis on acyclic polyenes [6], alkanes [8], and benzenoid hydrocarbons [7,10]. To our best knowledge, the spectral radius of graphs

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with $\kappa(G) \leq k$ was, so far, not considered in the chemical literature. On the other hand, graphs with $\kappa(G) \leq k$ represent important classes of molecules. Here we are concerned about graphs with $\kappa(G) \leq k$.

In order to describe our results, we need some graph-theoretic notation and terminology. Other undefined notations may be referred to [2].

Let $G = (V, E)$ be a simple undirected graph. For $v \in V(G)$, let $N_G(v)$ (or $N(v)$ for short) be the set of all neighbors of v in G and let $d(v) = |N(v)|$ be the degree of v. Let $e \notin E(G)$. We use $G + e$ to denote the graph obtained by adding e to G. For any set W of vertices (edges), $G - W$ and $G + W$ are the graphs obtained by deleting the vertices (edges) in W from G and adding the vertices (edges) in W to G, respectively. If G is connected and $G - W$ is disconnected, then we say that W is a *w-vertex* (*-edge*) *cut* of G where $w = |W|$. Other undefined notations may be referred to [2].

For $k \geq 1$, we say that a graph G is *k-connected* if either G is a complete graph K_{k+1}, or else it has at least $k+2$ vertices and contains no $(k-1)$-vertex cut. Similarly, for $k \geq 1$, a graph is a *k-edge-connected* if it has at least two vertices and does not contain $(k - 1)$-edge cut. The maximal value of k for which a connected graph G is k-connected is the *connectivity* of G, denoted by $\kappa(G)$. If G is disconnected, we define $\kappa(G) = 0$. The *edge-connectivity* $\kappa'(G)$ is defined analogously. If G is a graph of order n, we may have the following remarks.

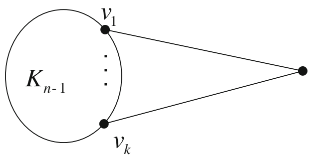
(1) $\kappa(G) \leq \kappa'(G) \leq n - 1$, and
(2) $\kappa(G) = n - 1$, $\kappa'(G) = n - 1$ and $G \cong K_n$ are equivalent.

We denote by $\mathcal{V}_n^k$ the set of graphs of order n with $\kappa(G) \leq k \leq n-1$, and by $\mathcal{E}_n^k$ the set of graphs of order n with $\kappa'(G) \leq k \leq n-1$. The graph K_n^k is a graph obtained by joining k edges from k vertices of K_{n-1} to an isolated vertex as shown in Fig. 1. It is obvious that $K_n^k \in \mathcal{E}_n^k \subseteq \mathcal{V}_n^k$. The graph G_n^k is a graph obtained by joining k isolated vertices to one vertex of K_{n-k}, and $G_{n,k}$ is obtained by adding a path of length l or $l + 1$ to each of the vertices of K_{n-k} for some positive integer l so that the order of $G_{n,k}$ is n.

Let $A(G)$ be the adjacency matrix of a graph G. The spectral radius, $\rho(G)$, of G is the largest eigenvalues of $A(G)$. For the results on the spectral radius of graphs, readers may refer to [1,13,17] and the references therein. If G is connected, $A(G)$ is irreducible and by the Perron-Frobenius Theorem, the spectral radius is simple and has a unique positive eigenvector (i.e., all entries of the vector are positive). We will refer to such an eigenvector as the *Perron vector of G*.

In [3], Brualdi and Solheid proposed the following problem concerning spectral radius:

Fig. 1 The graph K_n^k



Given a set of graphs $\Im$, find an upper bound for the spectral radius of graphs in $\Im$ and characterize the graphs in which the maximal spectral radius is attained.

Berman and Zhang [1] studied this question for graphs with n vertices and k cut vertices, and get the following result.

Theorem 1.1 *Among all the connected graphs of order n containing k cut vertices, the maximal spectral radius is obtained uniquely at $G_{n,k}$.*

Liu, Lu and Tian [13] studied the same question for graphs with n vertices and k cut edges, and get the following result.

Theorem 1.2 *Among all the connected graphs of order n containing k cut edges, the maximal spectral radius is obtained uniquely at G_n^k.*

In this paper, we investigate the problem for the graphs in $\Im = \mathcal{V}_n^k$, and in $\Im = \mathcal{E}_n^k$. We show that among all those graphs, the maximal spectral radius is obtained uniquely at K_n^k.

2 Main results

To obtain our main results, we will make use of the following lemmas.

Lemma 2.1 **([11])** *If G is a graph of order n and size m with no isolated vertices,*

$$\rho(G) \leq \sqrt{2m - n + 1}$$

with equality if and only if G is a star or the complete graph plus copies of K_2.

Lemma 2.2 **([17])** *Let G be a connected graph with vertices set $V = \{v_1, v_2, \ldots, v_n\}$. Let $u, v \in V$. Suppose $v_1, v_2, \ldots, v_s \in N(v) \setminus N(u)$ $(1 \leq s \leq d(v))$ and $[\mathbf{x}] = (x_1, x_2, \ldots, x_n)$ is the Perron vector of $A(G)$, where x_i corresponds to the vertex v_i. Let G^* be the graph obtained by deleting from G the edges vv_i $(1 \leq i \leq s)$, and then adding to G the edges uv_i $(1 \leq i \leq s)$. If $x_u \geq x_v$. Then $\rho(G) < \rho(G^*)$.*

Lemma 2.3 **([12,18])** *Let G be a connected graph, and G' be a proper subgraph of G. Then $\rho(G') < \rho(G)$.*

Corollary 2.4 *Let G be a graph and let $G+e$ be the graph obtained from G by adding a new edge e into G. Then $\rho(G) < \rho(G+e)$.*

In fact, suppose H is a subgraph of G. Then $\rho(H) \leq \rho(G)$.

Theorem 2.5 *Among all the graphs in $\mathcal{V}_n^k$, the maximal spectral radius is obtained uniquely at K_n^k.*

Proof We have to prove that for every $G \in \mathcal{V}_n^k$, then $\rho(G) \leq \rho(K_n^k)$, where the equality holds if and only if $G \cong K_n^k$. Since K_n^{n-1} $(\cong K_n)$ is the only graph in $\mathcal{V}_n^{n-1}$, the theorem holds when $k = n-1$. For $1 \leq k \leq n-2$, we let G^* with $V(G^*) = \{v_1, v_2, \ldots, v_n\}$ be the graph with the maximal spectral radius in $\mathcal{V}_n^k$; i.e. $\rho(G) \leq \rho(G^*)$ for all $G \in \mathcal{V}_n^k$.

Denote the Perron vector of $A(G^*)$ by $\mathbf{[x]} = (x_1, x_2, \ldots, x_n)$, where x_i corresponds to the vertex v_i $(i = 1, 2, \ldots, n)$. Since $G^* \in \mathcal{V}_n^k$ and G^* is not a complete graph, G^* has a k-vertex cut. Without loss of generality, we may let $V_1 = \{v_1, v_2, \ldots, v_k\}$ be a k-vertex cut of G^*. In the following, we will prove three claims.

Claim 1 *There are exactly two components of* $G^* - V_1$.

Suppose contrary that $G^* - V_1$ contains three components G_1, G_2 and G_3. Let $u \in G_1$ and $v \in G_2$. It is obvious that V_1 is also a k-vertex cut of $G^* + uv$; i.e. $G^* + uv \in \mathcal{V}_n^k$. By Corollary 2.4, we have $\rho(G^*) < \rho(G^* + uv)$. This contradicts the definition of G^*.

Therefore, $G^* - V_1$ has exactly two components G_1 and G_2.

Claim 2 *Each subgraph of* G^* *induced by vertices* $V(G_i) \cup V_1$, $i = 1, 2$, *is a clique.*

Suppose contrary that there is a pair of nonadjacent vertices $u, v \in V(G_i) \cup V_1$ for $i = 1$ or 2. Again, $G^* + uv \in \mathcal{V}_n^k$. By Corollary 2.4, we have $\rho(G^*) < \rho(G^* + uv)$. This contradicts the definition of G^*.

From Claim 2, it is clear that all G_1 and G_2 are cliques too. Then we write K_{n_i} instead of G_i, for $i = 1, 2$, in the rest of the proof, where $n_i = |G_i|$.

Claim 3 *Either* $n_1 = 1$ *or* $n_2 = 1$.

Otherwise, we have $n_1 > 1$ and $n_2 > 1$. Let $u \in K_{n_1}$ and $w \in K_{n_2}$. Suppose

$$N_{G^*}(u) = \{u_1, u_2, \ldots, u_{n_1 - 1}, v_1, v_2, \ldots, v_k\}$$

and

$$N_{G^*}(w) = \{w_1, w_2, \ldots, w_{n_2 - 1}, v_1, v_2, \ldots, v_k\}.$$

Let $G = G^* - \{ww_1, ww_2, \ldots, ww_{n_2-1}\} + \{uw_1, uw_2, \ldots, uw_{n_2-1}\}$ if $x_u \geq x_w$; otherwise, let $G = G^* - \{uu_1, uu_2, \ldots, uu_{n_1-1}\} + \{wu_1, wu_2, \ldots, wu_{n_1-1}\}$. In each of the above cases, $G \in \mathcal{V}_n^k$. By Lemma 2.2, $\rho(G^*) < \rho(G)$, which is a contradiction.

Hence $G^* \cong K_n^k$. This completes the proof. □

When $k = 1$, $\mathcal{V}_n^1$ is the set of all connected graphs of order n with a cut vertex. It is easy to get the following corollary.

Corollary 2.6 **([1])** *Among all connected graphs of order n with a cut vertex, the maximal spectral radius is obtained uniquely at* $K_n^1 \cong G_{n,1}$.

Since $K_n^k \in \mathcal{E}_n^k \subseteq \mathcal{V}_n^k$, the following corollary is obvious.

Corollary 2.7 *Among all the graphs in* $\mathcal{E}_n^k$, *the maximal spectral radius is obtained uniquely at* K_n^k.

When $k = 1$, $\mathcal{E}_n^1$ is the set of all connected graphs of order n with a cut edge. It is easy to get the following corollary.

Corollary 2.8 **([13])** *Among all connected graphs of order n with a cut edge, the maximal spectral radius is obtained uniquely at* $K_n^1 \cong G_n^1$.

Finally, we will illustrate some facts about $\rho(K_n^k)$:

Lemma 2.9 *The spectral radius* ρ *of the graph* K_n^k *satisfies the equation*

$$\rho^3 - (n-3)\rho^2 - (n+k-2)\rho + k(n-k-2) = 0. \tag{2.1}$$

Proof We assume that the vertex set of K_n^k is $\{v_0, v_1, \ldots, v_{n-1}\}$ (see Fig. 1), $\{v_0, v_1\}$, $\{v_0, v_2\}, \ldots, \{v_0, v_k\}$ are k edges adjacent to vertex v_0 in K_n^k. Let $(x_0, x_1, \ldots, x_{n-1})$ be the Perron vector of K_n^k, where x_i corresponds to the vertex v_i $(i = 0, 1, \ldots, n-1)$. By the symmetry of K_n^k, we have

$$x_1 = x_2 = \cdots = x_k \quad \text{and} \quad x_{k+1} = x_{k+2} = \cdots = x_{n-1}.$$

Setting $x_0 = x, \quad x_1 = y, \quad x_n = z$, we have

$$\begin{cases} \rho x = ky, \\ \rho y = x + (k-1)y + (n-k-1)z, \\ \rho z = ky + (n-k-2)z. \end{cases}$$

Hence,

$$z = \frac{[\rho - (k-1)]y - x}{n-k-1} = \frac{\rho - (k-1) - \frac{k}{\rho}}{n-k-1} y$$

and

$$z = \frac{k}{\rho - (n-k-2)} y.$$

So

$$\frac{\rho - (k-1) - \frac{k}{\rho}}{n-k-1} = \frac{k}{\rho - (n-k-2)},$$

and the result follows from the above equation. □

Corollary 2.10 *Let* ρ *be the spectral radius of the graph* K_n^k. *Then,*

$$\rho(K_n^k) < n - 2 + \frac{k^2}{(n-2)^2 - 1}.$$

Moreover, if k is fixed, then

$$\lim_{n \to \infty} [\rho - (n-2)] = 0.$$

Proof Since K_n^k contains a complete subgraph of order $n-1$, then $\rho > n-2$. Let $\rho = n-2+x$, where $x > 0$, substituting into Eq. 2.1. Then x satisfies the following equation:

$$x^3 + [2(n-2)+1]x^2 + [(n-2)^2 + (n-2) - k]x - k^2 = 0.$$

Assume $x_1 \geq x_2 \geq x_3$ are their roots, then we have

$$x_1 + x_2 + x_3 = -[2(n-2)+1], \tag{2.2}$$
$$x_1 x_2 x_3 = k^2, \tag{2.3}$$
$$x_1x_2 + x_1x_3 + x_2x_3 = (n-2)^2 + (n-2) - k. \tag{2.4}$$

It is easy to see that $x_1 > 0,\ x_2 < 0,\ x_3 < 0$ from Eqs. 2.2 and 2.3. From Eq. 2.4, we have

$$\begin{aligned} x_2x_3 &= (n-2)^2 + (n-2) - k - x_1(x_2+x_3) \\ &> (n-2)^2 + (n-2) - k \\ &\geq (n-2)^2 - 1. \end{aligned}$$

Then $x_1 = \dfrac{k^2}{x_2x_3} < \dfrac{k^2}{(n-2)^2-1}$. Hence $x < \dfrac{k^2}{(n-2)^2-1}$. The result holds. □

Remark 1 By Lemma 2.1, we have an upper bound of $\rho(K_n^k)$ as follows,

$$\rho(K_n^k) \leq \sqrt{n(n-1) - 2(n-1-k) - (n-1)} = \sqrt{(n-2)^2 + 2k - 1}. \tag{2.5}$$

For comparing with the bound described in Corollary 2.10, we consider the following quantity:

$$k^4 + 2(n-2)[(n-2)^2 - 1]k^2 - 2[(n-2)^2-1]^2k + [(n-2)^2-1]^2.$$

For convenience, we write $q = n-2$. Let

$$f(k) = k^4 + 2q(q^2-1)k^2 - 2(q^2-1)^2k + (q^2-1)^2, \text{ for } q \geq 3.$$

We have

$$\begin{aligned} f(0) &= (q^2-1)^2 > 0. \\ f(1) &= -q[(q^2-2)(q-2)-2] < 0. \\ f(q-2) &= -2q\big\{q[(q-4)(q+3)+1]+21\big\} + 21 < 0. \\ f(q-1) &= 4(q-1)^2 > 0. \end{aligned}$$

Since $f'(k) = 4k^3 + 4q(q^2-1)k - 2(q^2-1)^2$ and $f''(k) = 12k^2 + 4q(q^2-1) > 0$, $f(k)$ has only one minimum point. Thus $f(k) < 0$ when $1 \leq k \leq n-4$.

So the bound described in Corollary 2.10 is better than that described in (2.5) when $1 \leq k \leq n-4$.

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