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ON THE INDEX OF TRICYCLIC HAMILTONIAN GRAPHS

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Among the tricyclic Hamiltonian graphs with a prescribed number of vertices, the unique graph with maximal index is determined. Some subsidiary results are also included.

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1. Introduction

All multigraphs considered in this paper are finite and undirected. A multigraph without loops or multiple edges is called a graph. The *spectrum* of a graph G is the spectrum of a real $(0,1)$-adjacency matrix of G, and the largest eigenvalue of such a matrix is called the *index* of G, here denoted by $\mu(G)$. A graph with n vertices is *tricyclic* if it is connected and has $n+2$ edges.

A central part of algebraic graph theory is concerned with relations between the structure of a graph and its spectrum. Given a class $\mathscr{G}$ of graphs, one problem is to determine the graphs in $\mathscr{G}$ with maximal index. This problem has been solved when (for example) $\mathscr{G}$ consists of (i) all graphs with a prescribed number of edges [7], (ii) all unicyclic graphs with a prescribed number of vertices [**10**], (iii) all bicyclic graphs with a prescribed number of vertices [**12**], (iv) all bicyclic Hamiltonian graphs with a prescribed number of vertices [**6, 9**]. Further results may be found in [**2, 3, 9, 11**]. Here (in Theorem 3.6) we determine the unique graph with maximal index in $\mathscr{G}_n$, the class of all tricyclic Hamiltonian graphs with n vertices ($n \geq 5$). (Note that $\mathscr{G}_n$ is empty for $n<4$, while $\mathscr{G}_4$ contains only the complete graph on 4 vertices.) We think of a graph G in $\mathscr{G}_n$ as an n-cycle to which two chords are added as edges: the maximal degree $\Delta(G)$ of G is 4 or 3 according as the two chords do or do not have a vertex in common. Some subsidiary results concerning the index of a tricyclic Hamiltonian graph G with $\Delta(G)=4$ are given in Lemmas 3.3, 3.4 and 3.5. A result which may be of independent interest is Proposition 2.4, which provides a formula for the characteristic polynomial of a graph obtained from two graphs by the coalescence of an edge.

2. Some preliminary results

Our first result shows that if G is a graph with maximal index in $\mathscr{G}_n$ than $\Delta(G)=4$.

Proposition 2.1. *If $G \in \mathscr{G}_n$, $n \geq 5$ and $\Delta(G)=3$ then there exists $G' \in \mathscr{G}_n$ such that $\Delta(G')=4$ and $\mu(G')>\mu(G)$.*

Proof. Suppose that the vertices of a Hamiltonian cycle Z in G are labelled $1,2,\ldots,n$ in cyclic order, and let A be the corresponding adjacency matrix of G. Suppose that the two chords of Z join h to i and j to k (h,i,j,k distinct). Since G is connected, A is irreducible [**1**, p. 18] and it follows from the theory of irreducible non-negative matrices [**4**, Ch. XIII] that A has a unique positive unit eigenvector $\mathbf{x}$ corresponding to the eigenvalue $\mu(G)$, say $\mathbf{x}=(x_1,\ldots,x_n)^T$. Without loss of generality, $x_i \leqq x_j$, $x_i \leqq x_h$ and $x_i \leqq x_k$. If h is not adjacent to j then let G' be the graph obtained from G by deleting the edge hi and adding the edge hj. Note that $\Delta(G')=4$. Let A' be the adjacency matrix of G' and let $\mu'=\mu(G')$, $\mu=\mu(G)$. We have $\mu'-\mu \geqq \mathbf{x}^TA'\mathbf{x}-\mathbf{x}^TA\mathbf{x}=2x_h(x_j-x_i)\geqq 0$. If $\mu'=\mu$ then $\mathbf{x}^TA'\mathbf{x}=\mu'$ and $A'\mathbf{x}=\mu\mathbf{x}=A\mathbf{x}$; this is a contradiction because $A'\mathbf{x}$ has ith component $x_{i-1}+x_{i+1}$ (suffices reduced modulo n) while $A\mathbf{x}$ has ith component $x_{i-1}+x_{i+1}+x_h$. Thus $\mu'>\mu$ and the result is proved when h and j are non-adjacent.

Now suppose that h and j are adjacent. If h is not adjacent to k then we may repeat the above argument, this time obtaining G' by replacing hi by hk. Accordingly it suffices to deal with the case in which j, h, k are consecutive points of Z. Without loss of generality, $k=1$, $h=2$ and $j=3$. Since $n \geqq 5$ we may assume that $i \neq n$. Now let G' be obtained from G by replacing $2i$ with $1i$. Let $\mathbf{x}'$ be the unique positive unit eigenvector of A' corresponding to μ', say $\mathbf{x}'=(x'_1,\ldots,x'_n)^T$. We have $\mu'x'_1=x'_2+x'_3+x'_i+x'_n$ and $\mu'x'_2=x'_1+x'_3$, whence

$$\frac{x'_1-x'_2}{x'_i}=\frac{1}{\mu'+1}\left(1+\frac{x'_n}{x'_i}\right).$$

Further, $\mu x_1=x_2+x_3+x_n$ and $\mu x_2=x_1+x_3+x_i$, whence

$$\frac{x_2-x_1}{x_i}=\frac{1}{\mu+1}\left(1-\frac{x_n}{x_i}\right).$$

If $\mu'\leqq\mu$ then $(x'_1-x'_2)/x'_i>(x_2-x_1)/x_i$: this is a contradiction because $\mathbf{x}^T\mathbf{x}'(\mu'-\mu)=\mathbf{x}^TA'\mathbf{x}'-\mathbf{x}^TA\mathbf{x}'=x_i(x'_1-x'_2)-x'_i(x_2-x_1)$. Hence $\mu'>\mu$ and the proposition is proved.

In order to deal with the case $\Delta(G)=4$ ($G\in\mathcal{G}_n$) we shall need the following observations, where $\phi_H(x)$ denotes the characteristic polynomial of the multigraph H and $H-u$ denotes the multigraph obtained from H by deleting u and all edges containing u.

Lemma 2.2. *Let H, K be multigraphs, each with more than one vertex. If $H\cap K$ consists of the single vertex u then $\phi_{H\cup K}(x)=\phi_H(x)\phi_{K-u}(x)+\phi_{H-u}(x)\phi_K(x)-x\phi_{H-u}(x)\phi_{K-u}(x)$.*

Proof. For graphs, this is Corollary 2b of [**8**]. For a proof in the more general context, note that with a suitable labelling of vertices, $\phi_{H\cup K}(x)$ has the form

$$\begin{vmatrix} xI-A & \mathbf{r} & 0 \\ \mathbf{r}^T & x-a-b & \mathbf{s}^T \\ 0 & \mathbf{s} & xI-B \end{vmatrix}$$

which can be expanded as

$$\begin{vmatrix} xI-A & \mathbf{r} & 0 \\ \mathbf{r}^T & x-a & \mathbf{s}^T \\ 0 & \mathbf{0} & xI-B \end{vmatrix} + \begin{vmatrix} xI-A & \mathbf{0} & 0 \\ \mathbf{r}^T & x-b & \mathbf{s}^T \\ 0 & \mathbf{s} & xI-B \end{vmatrix} - \begin{vmatrix} xI-A & \mathbf{0} & 0 \\ \mathbf{r}^T & x & \mathbf{s}^T \\ 0 & \mathbf{0} & xI-B \end{vmatrix}.$$

The multigraph $H \cup K$ in Lemma 2.2 is said to be obtained from H and K by the *coalescence* of a vertex. We use the deletion-contraction algorithm (Lemma 2.3) to derive an analogous formula for graphs obtained by the coalescence of an edge (Proposition 2.4).

Lemma 2.3. *Let G be a finite multigraph with at least three vertices, let u, v be distinct vertices of G and let m be the number of edges between u and v. Let $G-uv$ be the multigraph obtained from G by deleting all m edges between u and v, and let G^* be the multigraph obtained from $G-uv$ by amalgamating u and v. Then*

$$\phi_G(x) = \phi_{G-uv}(x) + m\phi_{G^*}(x) + m(x-m)\phi_{G-u-v}(x) - m\phi_{G-u}(x) - m\phi_{G-v}(x).$$

Proof. [6, Theorem 1.3].

Proposition 2.4. *Let H, K be graphs, each with at least three vertices. If $H \cap K$ consists of the single edge uv (together with the vertices u and v) then*

$$\phi_{H\cup K}(x) = \phi_{(H\cup K)-uv}(x) + \phi_{H-u-v}(x)\phi_{K-u-v}(x)$$
$$+ \phi_{H-u-v}(x)\{\phi_K(x) - \phi_{K-uv}(x)\} + \phi_{K-u-v}(x)\{\phi_H(x) - \phi_{H-uv}(x)\}.$$

Proof. In what follows, an asterisk denotes a multigraph obtained by amalgamating u and v after deleting the edge uv. We first apply Lemma 2.3 to $H \cup K$ and the edge uv. We then apply Lemma 2.2 to (i) the coalescence of H^* and K^* at the amalgamated point u, (ii) the coalescence of $H-u$ and $K-u$ at v, (iii) the coalescence of $H-v$ and $K-v$ at u. We obtain

$$\phi_{H\cup K}(x) = \phi_{(H\cup K)-uv}(x)$$
$$+ \phi_{H^*}(x)\phi_{K-u-v}(x) + \phi_{K^*}(x)\phi_{H-u-v}(x)$$
$$- \phi_{H-u-v}(x)\phi_{K-u-v}(x) - \phi_{H-u}(x)\phi_{K-u-v}(x) - \phi_{K-u}(x)\phi_{H-u-v}(x)$$
$$- \phi_{H-v}(x)\phi_{K-u-v}(x) - \phi_{K-v}(x)\phi_{H-u-v}(x) + 2x\phi_{H-u-v}(x)\phi_{K-u-v}(x).$$

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The result follows by applying Lemma 2.3 to (i) H and the edge uv, (ii) K and the edge uv, and eliminating $\phi_{H^*}(x)$, $\phi_{K^*}(x)$.

For integers $h \geqq 1$, $t \geqq 0$, $k \geqq 1$ we define a graph $G(h,t,k)$ as follows. Let $n = h+t+k+3$ and let Z be the n-cycle $123\ldots n1$: the graph $G(h,t,k)$ is obtained from Z by adding edges joining 1 to $h+2$ and 1 to $n-k$. Thus $G(h,t,k) \in \mathscr{G}_n$ and $G(h,t,k)$ is a union of cycles of lengths $h+2$, $t+3$, $k+2$. Let $\mu(h,t,k)$ denote the index of $G(h,t,k)$.

Lemma 2.5. *$\mu(h,t,k) > \sqrt{5}$ for all $h \geqq 1$, $t \geqq 0$, $k \geqq 1$.*

Proof. By [**6**, Theorem 2.6], every bicyclic Hamiltonian graph on an even number of vertices has index $>\sqrt{5}$. The same is true of such graphs with an odd number of vertices because the index of such a graph decreases on subdivision of any edge [**5**, Proposition 2.4]. Since $G(h,t,k)$ has a bicyclic Hamiltonian subgraph, the result follows [**1**, Theorem 0.7].

Finally, we shall use implicitly the facts that the characteristic polynomial of an n-vertex path P_n is $U_n(\frac{1}{2}x)$, and the characteristic polynomial of an n-cycle C_n is $2T_n(\frac{1}{2}x)-2$ [**1**, p. 73]. Here T_n, U_n are Chebyshev polynomials of the first and second kind respectively: thus if $x = 2\cos\theta$ and $0 < \theta < \pi$ then $T_n(\frac{1}{2}x) = \cos n\theta$ and $U_n(\frac{1}{2}x) = \sin(n+1)\theta/\sin\theta$.

3. The main result

For integers $a \geqq 1$, $b \geqq 1$ we define a graph $H(a,b)$ as follows. Let $n = a+b+2$ and let Z be the n-cycle $123\ldots n1$: the graph $H(a,b)$ is obtained from Z by adding an edge joining 1 to $a+2$. Thus $H(a,b)$ is a union of cycles of lengths $a+2$, $b+2$. In what follows, we simplify notation by identifying a graph with its characteristic polynomial.

Lemma 3.1. *When $a \geqq 1$ and $b \geqq 1$ we have*

$$H(a,b) = C_{a+b+2} + C_{a+1}P_b + C_{b+1}P_a - P_aP_b - 2P_{a+b+1}.$$

Proof. First apply Lemma 2.3 to $H(a,b)$ and the edge joining 1 to $a+2$; secondly apply Lemma 2.2 to the coalescence (at a vertex) of cycles of lengths $a+1$ and $b+1$.

Lemma 3.2. *When $h \geqq 1$, $t \geqq 0$, $k \geqq 1$ and $n = h+t+k+3$ we have*

$$\begin{aligned} G(h,t,k) = C_n - 2P_{n-1} &+ P_{n-h-2}(C_{h+2} - P_{h+2}) \\ &+ P_h(P_{n-h-2} + C_{n-h} - 2P_{n-h-1}) \\ &+ P_h(C_{t+2}P_k + C_{k+1}P_{t+1} - P_kP_{t+1} - C_{k+2}P_{t+1} + P_{k+1}P_t) \\ &+ C_{h+t+2}P_k + C_{k+1}P_{h+t+1} - P_{h+t+1}P_k. \end{aligned}$$

Proof. Let $C_a * P_b$ denote the graph obtained by coalescence of a vertex of C_a with an end-vertex of P_b. Applying Proposition 2.4 to $G(h,t,k)$ and the edge joining 1 to $h+2$ we obtain

$$G(h,t,k)=H(h+t+1,k)+P_hP_{k+t+1}+P_{k+t+1}(C_{h+2}-P_{h+2})$$
$$+P_h(H(t+1,k)-C_{k+2}*P_{t+2}). \qquad (1)$$

Two applications of Lemma 2.2 yield the equation $C_{k+2}*P_{t+2}=C_{k+2}P_{t+1}-P_{k+1}P_t$. The result follows by applying Lemma 3.1 to $H(h+t+1,k)$ and $H(t+1,k)$.

Lemma 3.3. *If* $1\leqq k\leqq t$ *then* $\mu(h,t,k)<\mu(h,k-1,t+1)$.

Proof. By Lemma 3.2, $G(h,t,k)-G(h,k-1,t+1)=s_1+s_2+s_3+s_4$, where

$$s_1=C_{h+t+2}P_k+C_{k+1}P_{h+t+1}-C_{h+k+1}P_{t+1}-C_{t+2}P_{h+k},$$

$$s_2=P_{h+k}P_{t+1}-P_{h+t+1}P_k,$$

$$s_3=P_h(P_{k+1}P_t-P_{t+2}P_{k-1}),$$

$$s_4=P_h(C_{t+3}P_k-C_{k+2}P_{t+1}).$$

On simplifying the corresponding expressions involving Chebyshev polynomials (with argument $\frac{1}{2}x$), we obtain:

$$s_1=2(U_{t+1}+U_{h+k}-U_k-U_{h+t+1}),$$

$$s_2=U_{h-1}U_{t-k},$$

$$s_3=xU_hU_{t-k},$$

$$s_4=2U_h(U_{t+1}-U_k)-xU_hU_{t-k}.$$

On using the relation $U_aU_b-U_{a+b}=U_{a-1}U_{b-1}$, we obtain $G(h,t,k)-G(h,k-1,t+1)=U_{h-1}U_{t-k}+2[U_{h-1}(U_t-U_{k-1})+(U_{t+1}-U_k)]$. Since this function is positive on $[2,\infty)$ and $\mu(h,t,k)>\sqrt{5}$, the result follows.

Lemma 3.4. *If* $k\geqq t\geqq 1$ *then* $\mu(h,t,k)<\mu(h,t-1,k+1)$.

Proof. We deal first with the case $k>t+h$. From equation (1) we have

$$G(h,t,k)-G(h,t-1,k+1)=H(h+t+1,k)-H(h+t,k+1)$$

$$+P_h[H(t+1,k)-H(t,k+1)]+P_h[C_{k+3}*P_{t+1}-C_{k+2}*P_{t+2}].$$

Let $\lambda(a,b)$ denote the index of $H(a,b)$. Since $k>t+h$ we have $\lambda(h+t,k+1)>\lambda(h+t+1,k)$ by [**9**, Theorem 1]. It follows that the polynomial $H(h+t+1,k)-H(h+t,k+1)$ is positive for $x\geqq\lambda(h+t+1,k)$, and hence for $x\geqq\mu(h,t,k)$ because $H(h+t+1,k)$ is a subgraph of $G(h,t,k)$. Similarly, $H(t+1,k)-H(t,k+1)$ is positive for $x>\mu(h,t,k)$. It is straightforward to show that the polynomial $C_{k+3}*P_{t+1}-C_{k+2}*P_{t+2}$ is equal to $2T_{k-t-1}(\frac{1}{2}x)+2[U_{t+1}(\frac{1}{2}x)-U_t(\frac{1}{2}x)]+U_{k-t+1}(\frac{1}{2}x)$, which is positive on $[2,\infty)$. Thus the polynomial $G(h,t,k)-G(h,t-1,k+1)$ is positive for $x\geqq\mu(h,t,k)$ and it follows that $\mu(h,t,k)<\mu(h,t-1,k+1)$.

Now suppose that $t+h\geqq k\geqq t\geqq 1$. By Lemma 3.2 we have $G(h,t,k)-G(h,t-1,k+1)=s_1+s_2+s_3+s_4$ where

$$s_1=C_{h+t+2}P_k+C_{k+1}P_{h+t+1}-C_{h+t+1}P_{k+1}-C_{k+2}P_{h+t},$$

$$s_2=P_h[(C_{t+2}P_k-C_{t+1}P_{k+1})+(C_{k+3}P_t-C_{k+2}P_{t+1})-(C_{k+2}P_t-C_{k+1}P_{t+1})],$$

$$s_3=P_h[(P_{k+1}P_t-P_{t+1}P_k)-(P_{t-1}P_{k+2}-P_tP_{k+1})],$$

$$s_4=P_{h+t}P_{k+1}-P_{h+t+1}P_k.$$

Define $V_m=U_{m+1}-U_m$ and $U_{-1}=0$. Routine calculations yield the following equations, where as usual all Chebyshev polynomials have argument $\frac{1}{2}x$: $s_1=2(V_k-V_{h+t})$, $s_2=-2U_hT_{k-t+1}+2U_hV_k$, $s_3=2U_hT_{k-t+1}$ and $s_4=U_{h+t-k-1}$. Thus

$$G(h,t,k)-G(h,t-1,k+1)=2(V_k-V_{h+t})+2U_hV_k+U_{h+t-k-1}.$$

Now $U_hV_k=V_{h+k}+U_{h-1}V_{k-1}$ and so

$$G(h,t,k)-G(h,t-1,k+1)=2(V_{h+k}-V_{h+t})+2V_k+2U_{h-1}V_{k-1}+U_{h+t-k-1}.$$

This polynomial is positive on $[2,\infty)$ and so again $\mu(h,t,k)<\mu(h,t-1,k+1)$ as required.

Lemma 3.5. *If* $2\leqq h\leqq k$ *then* $\mu(h,0,k)<\mu(h-1,0,k+1)$.

Proof. Let C_a*C_b denote the graph obtained by the coalescence of a vertex in C_a with a vertex in C_b. Let $H_2(a,b)$ denote the multigraph obtained from $H(a,b)$ by adding a second edge joining 1 to $a+2$. On applying Lemma 2.3 to $G(h,0,k)$ and the vertices $h+2$, $h+3$ we obtain

$$G(h,0,k)=C_{h+2}*C_{k+2}+H_2(h,k)+(x-1)P_{h+k+1}$$

$$-C_{k+2}*P_{h+1}-C_{h+2}*P_{k+1}.$$

On applying Lemma 2.3 to $H_2(h,k)$ and the vertices $1, h+2$ we obtain

$$H_2(h,k)=C_{h+k+2}+2C_{h+1}*C_{k+1}+2(x-2)P_hP_k-4P_{h+k+1}.$$

Four applications of Lemma 2.2 now yield the equation

$$\begin{aligned}G(h,0,k)=&C_{h+2}P_{k+1}+C_{k+2}P_{h+1}-(x+2)P_{h+1}P_{k+1}+C_{h+k+2}\\&+2C_{h+1}P_k+2C_{k+1}P_h-4P_hP_k+(x-5)P_{h+k+1}\\&-C_{k+2}P_h-C_{h+2}P_k+xP_hP_{k+1}+xP_{h+1}P_k.\end{aligned}$$

It follows after a little work that

$$G(h,0,k)-G(h-1,0,k+1)=4(T_{k+2}-T_{h+1})-(x+2)U_{k-h}.$$

Suppose that $k\geqq h+1$. Then for $x\geqq 2$ we have

$$G(h,0,k)-G(h-1,0,k+1)\geqq f_k(x),$$

where

$$f_k(x)=4[T_{k+2}(\tfrac{1}{2}x)-T_k(\tfrac{1}{2}x)]-(x+2)U_{k-2}(\tfrac{1}{2}x).$$

For $x\geqq 2$ we write $x=2\cosh\theta$ ($\theta\geqq 0$) to obtain

$$f_k(x)=\frac{2(1+\cosh\theta)\cosh(k+1)\theta}{\sinh\theta}s_k(\theta)$$

where $s_k(\theta)=\sinh 2\theta-\{1+2(\cosh\theta-1)^2\}\tanh(k+1)\theta$. Now $s_k(\theta)\geqq h(\theta)$ where $h(\theta)=\sinh 2\theta-\{1+2(\cosh\theta-1)^2\}$; and $h(\theta)>0$ for $\theta>\sinh^{-1}(\tfrac{1}{2})$. It follows that $f_k(x)>0$ for $x>\sqrt{5}$ and we deduce from Lemma 2.5 that $\mu(h,0,k)<\mu(h-1,0,k+1)$ when $k\geqq h+1$.

Finally consider the case $k=h$: here $G(h,0,k)-G(h-1,0,k+1)=g_k(x)$ where $g_k(x)=4[T_{k+2}(\tfrac{1}{2}x)-T_{k+1}(\tfrac{1}{2}x)]-x-2$. Now $g_{k+1}(x)-g_k(x)=4(x-2)T_{k+2}(\tfrac{1}{2}x)$, which is positive for $x>2$. Hence for $x>2$ we have $g_k(x)\geqq g_2(x)=2x^4-2x^3-8x^2+5x+2$. Since $g_2(x)>0$ for $x>\sqrt{5}$, we deduce as before that $\mu(h,0,k)<\mu(h-1,0,k+1)$.

Theorem 3.6. *Let G be a tricyclic Hamiltonian graph with n vertices, $n\geqq 5$. If the index of G is maximal (for fixed n) then G is isomorphic to the graph $G(1,0,n-4)$ defined above.*

Proof. By Proposition 2.1, G is isomorphic to some $G(h,t,k)$ with $h\geqq 1$, $t\geqq 0$, $k\geqq 1$ and $h+t+k=n-3$. Since $G(h,t,k)$ is isomorphic to $G(k,t,h)$ we may assume that $h\leqq k$. By Lemma 3.3, $t<k$; by Lemma 3.4, $t=0$; and by Lemma 3.5, $h=1$. The result follows.

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