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The inertia of unicyclic graphs and the implications for closed-shells

Sean Daugherty

Department of Computer Science, University of Victoria, Victoria, BC, Canada V8W 3P6

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Abstract

The *inertia* of a graph is an integer triple specifying the number of negative, zero, and positive eigenvalues of the adjacency matrix of the graph. A *unicyclic* graph is a simple connected graph with an equal number of vertices and edges. This paper characterizes the inertia of a unicyclic graph in terms of maximum matchings and gives a linear-time algorithm for computing it. Chemists are interested in whether the molecular graph of an unsaturated hydrocarbon is (properly) *closed-shell*, having exactly half of its eigenvalues greater than zero, because this designates a stable electron configuration. The inertia determines whether a graph is closed-shell, and hence the reported result gives a linear-time algorithm for determining this for unicyclic graphs.

AMS classification: 58C40; 92E10; 05C85; 05C70

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1. Introduction

The *inertia* of a graph is an integer triple specifying the numbers of negative, zero, and positive eigenvalues of the adjacency matrix of the graph. A *unicyclic* graph is a simple connected graph with an equal number of vertices and edges. Here we present a method of calculating the inertia of a unicyclic graph from its maximum matchings.

E-mail address: sdaughe@cs.uvic.ca

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Many articles have recently appeared about the eigenvalues of unicyclic graphs in the context of matchings. Topics for such articles include general analysis [1,2], the spectral radius [3], energy [4,5], largest eigenvalues [6], and nullity [7]. One paper [8] uses methods similar to those presented here to determine the nullity of a unicyclic graph, but not the number of positive and negative eigenvalues.

According to Hückel theory, the eigenvalues of a *chemical graph* (connected graph with maximum degree at most three) specify the allowed energies of the π molecular orbitals available for occupation by electrons. Such a graph or corresponding molecule is said to be (properly) *closed-shell* if exactly half of its eigenvalues are positive (requiring an even number of vertices), which indicates a stable π-system [9, p. 47]. The study of the inertia of chemical graphs and its relation to predicted stability has been present for at least 35 years [10], though the predictors of stability differ slightly from the ones presented here. A *closed-shell independent set* can be used to predict addend bonding locations. Such a set is an independent set in which the components induced by the vertices not in the set are all closed-shell. The search for maximum closed-shell independent sets on fullerenes [11] benefits from a fast method of determining whether or not induced subgraphs of a fullerene are closed-shell. Many such subgraphs are unicyclic and the closed-shell nature of a graph follows immediately from its inertia. These facts motivated the study of the inertia of unicyclic graphs here.

2. Notation

A unicyclic graph contains n vertices and hence n edges. Let C_q be the subgraph induced by the vertices of the unique q-cycle of a unicyclic graph. Then $G - V(C_q)$ is the vertex-deleted subgraph created by removing the vertices of C_q and their incident edges.

Let A be the adjacency matrix of G. Then the characteristic polynomial of G is $P_G(\lambda) = a_0\lambda^n + a_1\lambda^{n-1} + \cdots + a_n$, the characteristic polynomial of A. For any graph, $a_0 = 1$. The multiplicity of $\lambda = 0$ as a root of this polynomial is given by $n - i$ where i is the largest value such that a_i is non-zero.

Let $m(G)$ denote the size of the maximum matching of a graph G, counting edges. Hence $m(G) = n/2$ means G has a perfect matching. A matching using i edges ($0 \leqslant i \leqslant n/2$) is called an i-matching. Let $m_i(G)$ denote the number of i-matchings on G. By definition, $m_0(G) = 1$ for any G.

The inertia of a graph G, $\mathrm{In}(G) = (p_-, p_0, p_+)$, is a triple composed of the number of negative, zero, and positive eigenvalues of $A(G)$, respectively. The function $\mathrm{sgn}(x)$ is the standard signum function.

3. Inertia

The inertia of a unicyclic graph is completely determined by the size q of its cycle, characteristics of the maximum matchings and, in the case q is odd, the size of a maximum matching of $G - V(C_q)$. The details are given in the main result, Theorem 6, which we prove in this section. The approach for the proof is to determine the sign of a sufficient number of the coefficients a_i in the characteristic polynomial $P_G(\lambda)$. Descartes' sign rule may then be applied to find p_+, the number of positive eigenvalues. Along the way, we also discover p_0 and hence p_-. We will use two well-known theorems, the latter of which can be found in almost any book on the theory of equations, such as [12, p.124].

Theorem 1 [13, Theorem 1.3, p.32]. *Call an "elementary figure"*

(a) *the graph K_2, or*
(b) *a cycle C_q $(q \geqslant 3)$,*

and call a "basic figure" U any graph all of whose components are elementary figures. Let $\mathscr{U}_i$ denote the set of all basic figures contained in G having exactly i vertices. Define the "contribution" $b(E)$ of an elementary figure E by

$$b(K_2) = -1, \qquad b(C_q) = 2(-1)^{q+1}$$

and a basic figure U by

$$b(U) = \prod_{E \in U} b(E).$$

Then for $i > 0$,

$$a_i = (-1)^i \sum_{U \in \mathscr{U}_i} b(U).$$

Theorem 2 (Descartes' sign rule). *The number of positive roots of a polynomial $f(x) = f_0 x^n + f_1 x^{n-1} + \cdots + f_n$ with all real roots is equal to the number of sign changes of f_i proceeding from f_0 to f_n, ignoring $f_i = 0$.*

Descartes' sign rule may be applied to $P_G(\lambda)$ because A has all real eigenvalues since A is real and symmetric. We now begin our proof of the main result by finding the sign of the coefficients of $P_G(\lambda)$ with even index. Note that here and henceforth an edge "incident to the cycle" refers to such an edge that is not on the cycle.

Lemma 3. *If G is a unicyclic graph with cycle C_q, then for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$,*

$$\operatorname{sgn}(a_{2i}) = \begin{cases} (-1)^i & \text{if } q \equiv 0 \ (\operatorname{mod} 4),\ 0 < i \leqslant m(G), \textit{ and there exists an} \\ & \textit{i-matching containing an edge incident to the cycle}, \\ (-1)^i & \textit{if } q \equiv 0 (\operatorname{mod} 4) \textit{ and } i = 0, \\ (-1)^i & \textit{if } q \equiv 2 (\operatorname{mod} 4) \textit{ and } i \leqslant m(G), \\ (-1)^i & \textit{if } q \textit{ is odd and } i \leqslant m(G), \textit{ and} \\ 0 & \textit{otherwise}. \end{cases}$$

Proof. Trivially $a_0 = 1$, which is equal to the stated result $(-1)^i$ for any value of q since $m(G) \geqslant 0$.

Assume q is odd. Then any basic figure on an even number of vertices consists only of copies of K_2. Such a matching of $2i$ vertices exists only if $i \leqslant m(G)$. Therefore, for $i > m(G)$, no basic figure exists and so $\operatorname{sgn}(a_{2i}) = 0$. Otherwise, each basic figure contributes $(-1)^i$ to the sum for a_{2i}, so the we have $\operatorname{sgn}(a_{2i}) = (-1)^{2i}(-1)^i = (-1)^i$.

Assume q is even and $i \geqslant 1$. Since any even cycle can be decomposed into a matching, we again have $\operatorname{sgn}(a_{2i}) = 0$ when $i > m(G)$. Suppose $2i < q$, then any basic figure on $2i$ vertices only contains copies of K_2 and $\operatorname{sgn}(a_{2i}) = (-1)^i$, as before. Finally, suppose $q \leqslant 2i \leqslant 2m(G)$ so that some basic figures on $2i$ vertices contain C_q and $i - q/2$ copies of K_2 and some basic figures contain only i copies of K_2. Thus,

$$
\begin{aligned}
a_{2i} &= (-1)^{2i}(m_{i-q/2}(G - V(C_q))[2(-1)^{q+1}(-1)^{i-q/2}] + m_i(G)[(-1)^i]) \\
&= (-1)^i(2m_{i-q/2}(G - V(C_q))(-1)^{q/2+1} + m_i(G)).
\end{aligned}
$$

When $q \equiv 2 (\mathrm{mod}\, 4)$, this simplifies to show $\mathrm{sgn}(a_{2i}) = (-1)^i$. When $q \equiv 0 (\mathrm{mod}\, 4)$, this implies that $\mathrm{sgn}(a_{2i}) = (-1)^i \mathrm{sgn}(m_i(G) - 2m_{i-q/2}(G - V(C_q)))$. But $m_i(G) \geqslant 2m_{i-q/2}(G - V(C_q))$ since $2m_{i-q/2}(G - V(C_q))$ matchings of G of size i can be found by using the two matching in the cycle. Furthermore, $m_i(G) > 2m_{i-q/2}(G - V(C_q))$ only when there exists a matching of G of size i that uses an edge between C_q and $G - V(C_q)$. $\square$

We now simplify Lemma 3 by determining when it is possible to have $q \equiv 0 (\mathrm{mod}\, 4), i \leqslant m(G)$, and the existence of an i-matching containing an edge between C_q and $G - V(C_q)$.

Lemma 4. *For G a unicyclic graph with cycle C_q, let*

$$
k = \begin{cases} m(G) - 1 & \textit{if } q \equiv 0 \ (\mathrm{mod}\ 4) \textit{ and no maximum matching} \\ & \textit{contains an edge incident to the cycle, and} \\ m(G) & \textit{otherwise.} \end{cases}
$$

Then for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$,

$$
\mathrm{sgn}(a_{2i}) = \begin{cases} (-1)^i & \textit{if } i \leqslant k, \textit{ and} \\ 0 & \textit{otherwise.} \end{cases}
$$

Proof. The statement follows immediately from Lemma 3 except in the case where $q \equiv 0 (\mathrm{mod}\, 4)$ and $0 < i \leqslant m(G)$. For theremainder of the proof, we assume these two conditions and use them toprove that there exists an $m(G) - 1$ matching containing an edge incident to the cycle.

Notice that if an i-matching exists containing an edge incident to the cycle for $i > 1$ then such an $(i - 1)$-matching also exists. Likewise, if no i-matching exists containing an edge incident to the cycle then no$(i + 1)$-matching exists containing such an edge. Thus, there is some maximum value k such that there exists a k-matching containing an edge incident to the cycle, but no such $(k + 1)$-matching exists. Clearly, $k \leqslant m(G)$. Also, $k = 0$ if and only if $G = C_q$.

Suppose $0 < k < m(G)$. That is, no maximum matching contains an edge incident to the cycle. Consider a maximum matching M and an edge $e = (u, v)$ incident to the cycle such that $u \in V(C_q)$ and $v \notin V(C_q)$. Hence, for all such choices of M and e, $e \notin M$. Furthermore, since M is maximum and q is even, every vertex on thecycle is incident to a matched edge on the cycle, as shown in Fig. 1. Let f be the matched cycle edge incident to u. There also must exist an edge $g \in M$ incident to v, otherwise the matching $M - f + e$ would be a maximum matching that contradicts $k \neq m(G)$. Note that $M - f - g + e$ is a matching of size $m(G) - 1$ containing anedge incident to the cycle and hence $k = m(G) - 1$.

Finally, suppose $k = 0$ and hence $G = C_q$. The argument in the proof of Lemma 3 shows that $a_{2i} = (-1)^i$ for $2i < q$. When $2i = q$, there are exactly three basic figures: two perfect matchings andone containing only C_q. Direct application of Theorem 1 shows $a_q = 0$. $\square$

We will apply Theorem 2 to count the number of positive eigenvalues of A by counting the number of sign changes from a_0 to a_n. Lemma 4 shows that the coefficients a_{2i} begin at $a_0 = 1$ and alternate in sign, ending at a point where the remaining coefficients are all 0. Let k be the maximum value such that $a_{2k} \neq 0$. Then it does not matter what the values of a_{2i+1} are for $0 \leqslant i < k$, as they do not affect the number of sign changes since the sign of a_{2i+1} is either the

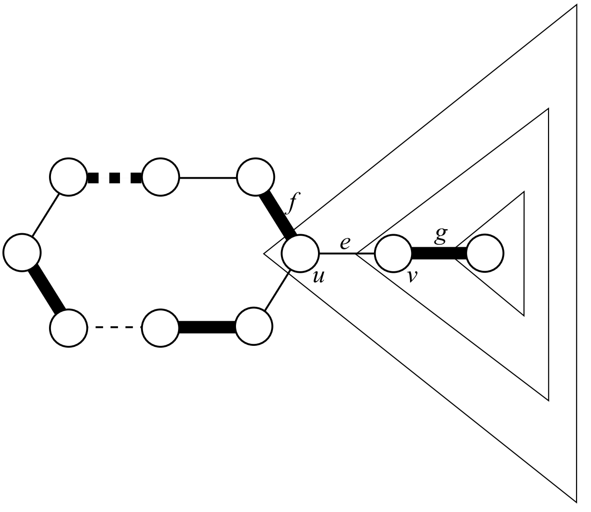

Fig. 1. A case considered in the proof of Lemma 4. Bold edges are in the maximum matching M. Triangles represent unknown tree-like parts of the graph. Tree-like additions are not restricted to u and may be attached to any other vertex on the cycle.

same as a_{2i} or a_{2i+2}, or $a_{2i+1} = 0$. Thus, we only consider the odd coefficients a_{2i+1} when $i \geqslant k$. We characterize those now.

Lemma 5. *Let G be a unicyclic graph with cycle C_q. Let k be the maximum value such that $a_{2k} \neq 0$. Then $a_{2i+1} = 0$ for all $i > k$.*

Proof. This is trivial in the case where q is even, because there exist no basic figures on an odd number of vertices. Assume q is odd. If there exists a basic figure on $2i + 1$ vertices, then there exists a basic figure on $2i$ vertices, which is found by replacing C_q (which must be included) in the basic figure with $(q - 1)/2$ copies of K_2 to get a matching of size i. Thus, $a_{2i+1} = 0$ for $i > k$. $\square$

Our search for the number of sign changes has now been reduced to finding the sign of a_{2k+1}. All the odd coefficients are 0 when q is even. The only case to consider is q odd, and recall that k has been defined in this case to equal $m(G)$. A basic figure on $2m(G) + 1$ vertices must contain C_q and $(2m(G) + 1 - q)/2$ copies of K_2 from $G - V(C_q)$. Therefore, we have

$$\begin{aligned} a_{2m(G)+1} &= (-1)^{2m(G)+1}(m_{m(G)-(q-1)/2}(G - V(C_q)))(2(-1)^{q+1}(-1)^{m(G)-(q-1)/2}) \\ &= -2(m_{m(G)-(q-1)/2}(G - V(C_q)))((-1)^{m(G)-(q-1)/2}). \end{aligned}$$

So,

$$\operatorname{sgn}(a_{2m(G)+1}) = \begin{cases} (-1)^{m(G)-(q-1)/2+1} & \text{if } q \text{ is odd and } m_{m(G)-(q-1)/2}(G - V(C_q)) > 0, \\ & \text{and} \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, $\operatorname{sgn}(a_{2m(G)+1})$ is the opposite of $\operatorname{sgn}(a_{2m(G)}) = (-1)^{m(G)}$ when $q \equiv 1 (\operatorname{mod} 4)$ and $m_{m(G)-(q-1)/2}(G - V(C_q)) > 0$. They have the same sign when $q \equiv 3 (\operatorname{mod} 4)$ and

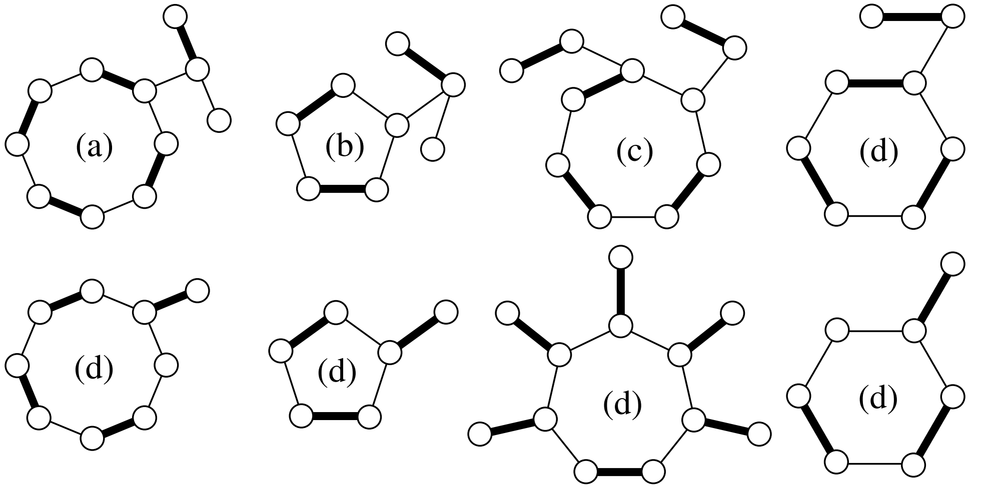

Fig. 2. Some unicyclic graphs, each labeled with the applicable case from Theorem 6 and an illustrative maximum matching. The inertia for each graph in clockwise order from the top left is: (4, 3, 4), (3, 1, 4), (6, 0, 5), (4, 0, 4), (3, 1, 3), (6, 0, 6), (3, 0, 3), (4, 1, 4).

$m_{m(G)-(q-1)/2}(G - V(C_q)) > 0$. The requirement $m_{m(G)-(q-1)/2}(G - V(C_q)) > 0$ means there exists a maximum matching of G that does not use any edge between C_q and $G - V(C_q)$. This is equivalent to $2m(G) + 1 = 2m(G - V(C_q)) + q$.

The number of positive eigenvalues can now be determined by counting the number of sign changes of the a_i's. The number of zero eigenvalues is $n - i$ where i is the largest value such that $a_i \neq 0$. The number of negative eigenvalues, and hence the inertia of a unicyclic graph, can then be computed by considering the size of a maximum matching of G and, if necessary, $G - V(C_q)$. From the above analysis we have proved the following.

Theorem 6. *For G, a unicyclic graph containing the cycle C_q*, $\mathrm{In}(G) = (p_-, p_0, p_+) =$

$$\begin{cases} \textbf{(a)}\ \ (m(G)-1, n-2m(G)+2, m(G)-1) & \textit{if } q \equiv 0 (\mathrm{mod}\, 4) \textit{ and no} \\ & \textit{maximum matching contains} \\ & \textit{an edge incident to } C_q, \\ \textbf{(b)}\ \ (m(G), n-2m(G)-1, m(G)+1) & \textit{if } q \equiv 1 (\mathrm{mod}\, 4) \textit{ and} \\ & 2m(G)+1 = 2m(G-V(C_q))+q, \\ \textbf{(c)}\ \ (m(G)+1, n-2m(G)-1, m(G)) & \textit{if } q \equiv 3 (\mathrm{mod}\, 4) \textit{ and} \\ & 2m(G)+1=2m(G-V(C_q))+q, \textit{ and} \\ \textbf{(d)}\ \ (m(G), n-2m(G), m(G)) & \textit{otherwise}. \end{cases}$$

Example graphs that illustrate the cases of Theorem 6 are shown in Fig. 2. Where multiple maximum matchings exist, a maximum matching is shown that illustrates the applicable case. The top row shows examples with a maximum matching that does not contain an edge incident to C_q and the bottom row shows examples with a maximum matching that does contain such an edge.

4. Inertia algorithm

It is possible to compute the inertia of a unicyclic graph in linear time using a simple variation of the Karp–Sipser leaf-removal algorithm [14]. The first phase of the algorithm repeatedly removes a leaf, its neighbor, and any incident edges from the graph. The edge incident to the leaf is added to the matching. It was shown that this phase of the algorithm makes no "mistakes." That is, a maximum matching of the remaining graph, the *core*, produces a maximum matching of the original graph when combined with the edges selected by the leaf-removal phase. The next phase of the algorithm involves selecting a random edge when no leaf exists then continuing again with leaf-removal. However, this is unnecessary for unicyclic graphs as discussed below.

In the case of unicyclic graphs, after leaf-removal one is left with a core of either (1) the null graph, (2) isolated vertices, or (3) the cycle and possibly some isolated vertices. In case (3), a maximum matching contains $\lfloor q/2 \rfloor$ more edges than were selected by the leaf-removal. To find the inertia when q is odd, the size of a maximum matching of the forest $G - V(C_q)$ can also be determined by the Karp–Sipser algorithm. In this case, it is easy to locate and remove C_q from G in linear time using a breadth-first search.

When $q \equiv 0 \pmod 4$, the algorithm can be used to determine if no maximum matching contains an edge incident to the cycle, since this occurs exactly when the algorithm results in case (3) above. The reason is as follows. Let $V(C_q) = \{v_1, v_2, \ldots v_q\}$, and let T_i be the maximal-sized tree rooted at v_i using no edges of the cycle. Finally, let t_i be the size of a maximum matching of T_i. Because the leaf removal is mistake-free, the algorithm accurately finds each t_i, regardless of the order in which the leaves are removed. Assuming that the algorithm found a maximum matching of G containing no edges incident to the cycle, it resulted in case (3). In that case, the size of a maximum matching of G is $t_1 + t_2 + \cdots + t_q + q/2$. If a different maximum matching of G (one not found by the algorithm) exists using an edge incident to the cycle, there cannot be $q/2$ cycle edges in the matching and so such a matching can have at most $t_1 + t_2 + \cdots + t_q + q/2 - 1$ edges, and therefore cannot also be maximum. Thus, when the algorithm results in case (3), no maximum matching exists containing an edge incident to the cycle.

The maximum matchings shown in Fig. 2 are examples of those that may be found by the inertia algorithm. Other matchings may be found, depending on the order in which leaves are selected for removal and the chosen matching of the remaining cycle in the event of case (3).

5. Closed-shells

Recall that a graph G is called *properly closed-shell* if n is even and exactly half of its eigenvalues are positive. It is easy to determine whether or not a unicyclic graph is closed-shell if the inertia is already known. However, if one is only concerned with whether or not a unicyclic graph is closed-shell and does not need to know the inertia, such a conclusion can be reached using less information than is required by Theorem 6.

Corollary 7. *Let G be a unicyclic graph with cycle C_q. Then G is closed-shell if and only if it has an even number of vertices and one of the following mutually-exclusive cases holds*:

Case 1. $q \equiv 0 \pmod 4$ *and G has a unique perfect matching*,
Case 2. $q \equiv 1 \pmod 4$ *and either*
  2.1. $2m(G) - 2m(G - V(C_q)) = q - 1$ *and* $m(G) = n/2 - 1$, *or*

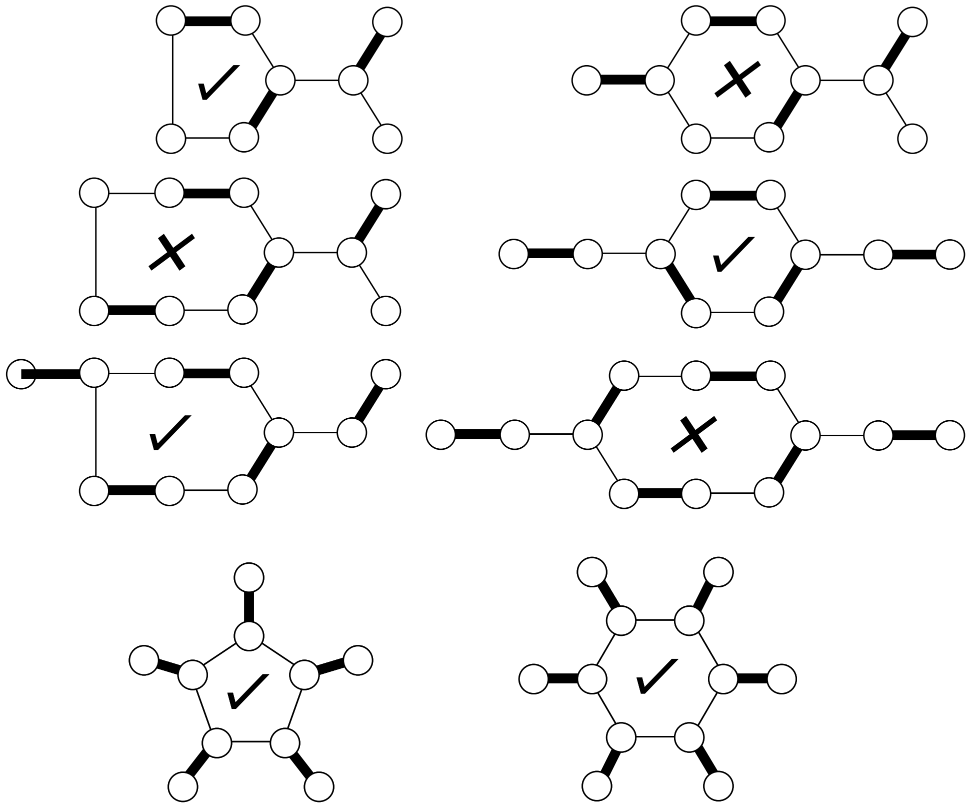

Fig. 3. Some unicyclic graphs, with a maximum matching of each shown in bold. Examples that are closed-shell are checked.

2.2. $2m(G) - 2m(G - V(C_q)) \neq q - 1$ *and G has a perfect matching*,
Case 3. $q \equiv 2(\text{mod}\, 4)$ *and G has a perfect matching*, *or*
Case 4. $q \equiv 3(\text{mod}\, 4)$ *and G has a perfect matching*.

Proof. Recall that a graph is closed-shell if and only if $p_+ = n/2$. For each value of $q(\text{mod}\, 4)$, we determine the conditions in which this holds true by considering the four cases of Theorem 6.

Case 1. $q \equiv 0(\text{mod}\, 4)$

Either case (a) or (d) applies from Theorem 6. A graph G cannot be closed-shell if case (a) applies since $p_+ = m(G) - 1 < n/2$. If case (d) applies, then $p_+ = m(G)$ so G is closed-shell if and only if it has at least one perfect matching. Case (d) applies only when some maximum matching contains an edge incident to C_q. Note that a unicyclic graph has at most two perfect matchings, which follows from the algorithm for calculating the inertia since only isolated vertices and the cycle may remain after leaf-removal. Furthermore, a perfect matching is unique if and only if it contains an edge incident to C_q (such that the cycle does not remain after leaf-removal). Therefore G is closed-shell if and only if it has a unique perfect matching.

Case 2. $q \equiv 1 (\mathrm{mod}\, 4)$

Either case (b) or (d) applies, so G is closed-shell if and only if it has a perfect matching (case (d)), unless $2m(G) + 1 = 2m(G - V(C_q)) + q$ (case (b)), in which case the requirement is that $m(G) + 1 = n/2$.

Case 3. $q \equiv 2 (\mathrm{mod}\, 4)$

Only case (d) applies, so G is closed-shell if and only if it has at least one perfect matching.

Case 4. $q \equiv 3 (\mathrm{mod}\, 4)$

Either case (c) or (d) applies and $p_+ = m(G)$ in each case so G is closed-shell if and only if it has at least one perfect matching. □

Examples of unicyclic graphs that are or are not closed-shell are given in Fig. 3. This includes some graphs that are not closed-shell yet contain a perfect matching and some graphs that are closed-shell yet have no perfect matching.

Clearly, determining if a unicyclic graph is closed-shell can also be computed in linear time. In many cases, this calculation can be performed slightly faster than it was for the general inertia. Repeated leaf removal can be used to determine the size of a maximum matching as well as the number of perfect matchings. When $q \equiv 1 (\mathrm{mod}\, 4)$ and $m(G) \geqslant n/2 - 1$, the size of a maximum matching of $G - V(C_q)$ must be determined to apply Corollary 7. This can be computed by running the Karp–Sipser algorithm on the forest $G - V(C_q)$.

Two early-termination conditions can be applied to the leaf removal algorithm because only perfect or near-perfect matchings are allowed for closed-shell unicyclic graphs. When $q \not\equiv 1 (\mathrm{mod}\, 4)$, a perfect matching is required and the algorithm can terminate with the answer "not closed-shell" when an isolated vertex appears. When $q \equiv 1 (\mathrm{mod}\, 4)$, the algorithm can terminate with the response "not closed-shell" when three isolated vertices appear, which implies $m(G) < n/2 - 1$.

When searching for the maximum size of a closed-shell independent set for fullerenes [11], unicyclic graphs often arise as induced subgraphs to be tested for closed-shell properties. Implementation of this linear time algorithm helped increase the speed of the backtracking search.

The study of closed-shell conditions of other classes of graphs that appear as induced subgraphs of fullerenes may also speed up the algorithm implementation or lead to insights about ways to calculate the closed-shell independence number of fullerenes without backtracking. Though a plethora of induced fullerene subgraph classes exists, focusing on simple classes such as bicyclic graphs and cacti may be rewarding. Simpler results may be possible by restricting the analysis to graphs that are planar, of maximum degree at most three, and/or of girth at least five.

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