Unicyclic graphs with maximal energy

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Abstract

Let $G$ be a graph on $n$ vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. The energy of $G$ is defined as $E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. For various classes of unicyclic graphs, the graphs with maximal energy are determined. Let $P_n^6$ be obtained by connecting a vertex of the circuit $C_6$ with a terminal vertex of the path $P_{n-6}$. For $n \geq 7$, $P_n^6$ has the maximal energy among all connected unicyclic bipartite $n$-vertex graphs, except the circuit $C_n$.

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1. Introduction

Let $G$ be a graph on $n$ vertices and let $A(G)$ be its adjacency matrix. The characteristic polynomial of $A(G)$,

$$\phi(G; \lambda) = \det(\lambda I - A(G)) = \sum_{i=0}^{n} a_i \lambda^{n-i},$$

for which

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where $I$ stands for the unit matrix of order $n$, is said to be the characteristic polynomial of the graph $G$. The $n$ roots of the equation $\phi(G; \lambda) = 0$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are the eigenvalues of the graph $G$. Since $A(G)$ is symmetric, all eigenvalues of $G$ are real.

In chemistry the (experimentally determined) heats of formation of conjugated hydrocarbons are closely related to the total $\pi$-electron energy (a theoretically calculated quantity). Within the framework of the so-called HMO model (see [8]) the total $\pi$-electron energy is calculated from the eigenvalues of a pertinently constructed “molecular” graph $G$ as

$$E(G) = \sum_{j=1}^{n} |\lambda_j|.$$  

The right-hand side of Eq. (2) is well defined for all graphs (no matter whether they represent molecules or not). Bearing this in mind, Eq. (2) can be viewed as the definition of a graph-theoretical quantity $E(G)$ called the energy of the graph $G$. For a survey of the mathematical properties of $E(G)$ see Chapter 12 of the book [8] and the recent review [7]. One of the long-known results in this field is the Coulson integral formula (see [7,8]):

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{j=0}^{\lceil n/2 \rceil} (-1)^j a_j x^{2j} \right)^2 + \left( \sum_{j=0}^{\lceil n/2 \rceil} (-1)^j a_{j+1} x^{2j+1} \right)^2 \right],$$

where $a_0, a_1, \ldots, a_n$ are the coefficients of the characteristic polynomial of $G$, as in Eq. (1).

Quite a few lower and upper bounds for $E(G)$ are known [7,8]. On the other hand, very little is known about graphs with extremal energy. Graphs with extremal energy have been determined only for $n$-vertex trees [5,10,12] and $n$-vertex trees with perfect matchings [11]. Recently the unicyclic graphs with minimal energy were characterized [9]. Concerning unicyclic graphs with maximal energy, Caporossi et al. [1] put forward the following conjecture.

Denote, as usual, the $n$-vertex path and circuit by $P_n$ and $C_n$, respectively. Let $P^\ell_n$ be the unicyclic graph obtained by connecting a vertex of $C_\ell$ with a terminal vertex of $P_{n-\ell}$ (see Fig. 1).

**Conjecture** ([1]). Among unicyclic graphs on $n$ vertices the circuit $C_n$ has maximal energy if $n \leq 7$ and $n = 9, 10, 11, 13$ and $15$. For all other values of $n$ the unicyclic graph with maximum energy is $P^6_n$. 

Fig. 1.

In what follows we prove a result which is weaker than the above conjecture, namely that \( E(P_6^4) \) is maximal within the class of connected unicyclic bipartite \( n \)-vertex graphs that differ from \( C_n \).

In this paper we consider only connected graphs. Let \( G(n, \ell) \) be the set of all connected unicyclic graphs on \( n \) vertices, containing as a subgraph the circuit \( C_\ell \). Let \( C(n, \ell) \) be the set of all unicyclic graphs obtained from \( C_\ell \) by adding to it \( n - \ell \) pendant vertices. Note that \( G(n, n) = C(n, n) = \{C_n\} \) and \( G(n, n - 1) = C(n, n - 1) = \{P_n^{n-1}\} \).

2. Graphs in \( G(n, \ell) \) with maximal energy

For an \( n \)-vertex graph \( G \) let \( b_i = b_i(G) = |a_i(G)|, i = 0, 1, \ldots, n \), where \( a_i \) are the coefficients of the characteristic polynomial, as in Eq. (1). Notice that \( b_0(G) = 1 \), \( b_1(G) = 0 \) and \( b_2(G) \) is the number of edges of \( G \). The number of \( k \)-matchings of \( G \) is denoted by \( m(G, k) \). If \( G \) is acyclic, then for \( k \geq 0, b_{2k} = m(G, k) \) and \( b_{2k+1} = 0 \). It is both consistent and convenient to define \( m(G, k) = 0 \) and \( b_k(G) = 0 \) for \( k < 0 \).

Our starting point is a result which is an immediate and well-known corollary of the Sachs theorem (see [4, Section 1.4]).

**Lemma 2.1.** If \( G \) is a unicyclic graph with a circuit of size \( \ell \), then for all \( k \geq 0, (-1)^k a_{2k} \geq 0. \) Further, \( (-1)^k a_{2k+1} \geq (\text{resp.} \leq) 0 \) if \( \ell = 2r + 1 \) and \( r \) is odd (resp. even).

By means of Lemma 2.1, formula (3) is reduced to

\[
E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{j=0}^{[n/2]} b_{2j} x^{2j} \right)^2 + \left( \sum_{j=0}^{[n/2]} b_{2j+1} x^{2j+1} \right)^2 \right].
\]  

(4)

Thus, in the case of unicyclic graphs \( E(G) \) is a monotonically increasing function of \( b_i(G), i = 1, 2, \ldots, n \). Consequently, if \( G_1 \) and \( G_2 \) are unicyclic graphs for which

\[
b_1(G_1) \geq b_1(G_2)
\]

(5)
holds for all $i \geq 0$, then
\[ E(G_1) \succeq E(G_2). \] (6)
Equality in (6) is attained only if (5) is an equality for all $i \geq 0$.

If relations (5) hold for all $i$, then we write $G_1 \succeq G_2$ or $G_2 \preceq G_1$. If $G_1 \succeq G_2$, but not $G_2 \succeq G_1$, then we write $G_1 > G_2$. Using this notation, we re-state the above result as follows.

**Lemma 2.2.** Let $G$ and $H$ be unicyclic graphs. Then $G \succeq H$ implies $E(G) \geq E(H)$, and $G > H$ implies $E(G) > E(H)$.

**Lemma 2.3.**

(a) Let $G \in G(n, \ell)$ with $\ell \not\equiv 0 \mod 4$. If $uv$ is an edge of $G$ belonging to the circuit $C_\ell$, then
\[ b_i(G) = b_i(G - uv) + b_{i-2}(G - v - u) + 2b_{i-\ell}(G - C_\ell). \] (7)

(b) Let $G \in G(n, \ell)$, and let $uv$ be a pendant edge of $G$ with the pendant vertex $v$. Then
\[ b_i(G) = b_i(G - v) + b_{i-2}(G - v - u). \] (8)

**Proof.** (a) The characteristic polynomial of any graph satisfies the recursion relation [4]
\[ \phi(G; \lambda) = \phi(G - uv; \lambda) - \phi(G - v - u; \lambda) - 2 \sum_Z \phi(G - Z; \lambda), \] (9)
with summation going over all circuits $Z$ which contain the edge $uv$. Thus,
\[ b_i(G) = |a_i(G)| = |a_i(G - uv) - a_{i-2}(G - v - u) - 2a_{i-\ell}(G - C_\ell)| \]
\[ = |a_i(G - uv)| + |a_{i-2}(G - v - u)| + 2|a_{i-\ell}(G - C_\ell)| \]
\[ = b_i(G - uv) + b_{i-2}(G - v - u) + 2b_{i-\ell}(G - C_\ell). \]

(b) Eq. (8) is deduced from
\[ \phi(G; \lambda) = \lambda \phi(G - v; \lambda) - \phi(G - v - u; \lambda). \]

**Lemma 2.4.** Let $G \in G(n, \ell)$ where $\ell \not\equiv 0 \mod 4$. If $G \neq P_n^\ell$ then $G < P_n^\ell$.

**Proof.** We prove the lemma by induction on $n - \ell$.

Case 1: $\ell$ is odd. In a trivial manner the lemma holds for $n - \ell = 0$ and $n - \ell = 1$, because then $G(n, \ell)$ has only a single element. Let $p \geq 2$ and suppose the result is true for $n - \ell < p$. Now we consider $n - \ell = p$. Since $G$ is unicyclic and not a circuit, for $n > \ell$, $G$ must have a pendant edge $uv$ with pendant vertex $v$. As $G \neq P_n^\ell$ and $n \geq \ell + 2$, we may choose a pendant edge $uv$ of $G$ such that $G - v \neq P_{n-1}^\ell$. By Lemma 2.3,
\[ b_i(G) = b_i(G - v) + b_{i-2}(G - v - u), \quad (10) \]
\[ b_i(P^n_\ell) = b_i(P^{\ell}_{n-1}) + b_{i-2}(P^{\ell}_{n-2}). \quad (11) \]

By the induction assumption, \( G - v \prec P^{\ell}_{n-1} \).

If \( G - v - u \) contains the circuit \( C_\ell \), then by the induction assumption, we have \( G - v - u \preceq P^{\ell}_{n-2} \). (It is easy to show that this relation holds also if \( G - u - v \) is not connected.) Thus the lemma follows from Eqs. (10), (11) and the inductive assumption.

If \( G - v - u \) does not contain the circuit \( C_\ell \), then it is acyclic. Then \( b_{i-2}(G - v - u) = 0 \) when \( i \) is odd whereas for \( i = 2k \),

\[ b_{2k-2}(G - v - u) = m(G - v - u, k - 1) \leq m(P^{\ell}_{n-2}, k - 1) \]
\[ < m(P^{\ell}_{n-2}, k - 1) = b_{2k-2}(P^{\ell}_{n-2}). \quad (12) \]

Lemma 2.4 now follows from Eqs. (10)–(12) and the inductive assumption.

**Case 2:** \( \ell \) is even, hence \( \ell = 4r + 2 \). In this case, all elements of \( G(n, \ell) \) are bipartite graphs and \( b_i(G) = 0 \) when \( i \) is odd. Evidently, the lemma holds when \( n - \ell = 0, 1 \). Let \( p \geq 2 \) and suppose the result is true for \( n - \ell < p \). Now we consider \( n - \ell = p \). Since for \( n > \ell \), \( G \) is unicyclic and not a circuit, \( G \) must have a pendant edge \( uv \) with pendant vertex \( v \). As \( G \neq P^{\ell}_n \) and \( n \geq \ell + 2 \), we may choose a pendant edge \( uv \) of \( G \) such that \( G - v \neq P^{\ell}_{n-1} \). By Lemma 2.3,

\[ b_{2k}(G) = b_{2k}(G - v) + b_{2k-2}(G - v - u), \quad (13) \]
\[ b_{2k}(P^n_\ell) = b_{2k}(P^{\ell}_{n-1}) + b_{2k-2}(P^{\ell}_{n-2}). \quad (14) \]

By the induction assumption, we have \( G - v \prec P^{\ell}_{n-1} \).

If \( G - v - u \) contains the circuit \( C_\ell \), then by the induction assumption, we have \( G - v - u \preceq P^{\ell}_{n-2} \). Thus the lemma follows from Eqs. (13), (14) and the inductive assumption.

If \( G - v - u \) does not contain the circuit \( C_\ell \), then it is acyclic. Thus \( b_{i-2}(G - v - u) = 0 \) when \( i \) is odd and when \( i = 2k \),

\[ b_{2k-2}(G - v - u) = m(G - v - u, k - 1) \]
\[ \leq m(P^{\ell}_{n-2}, k - 1) \]
\[ < m(P^{\ell}_{n-2}, k - 1) \]
\[ \leq m(P^{\ell}_{n-2}, k - 1) + 2m(P^{\ell}_{n-2}, k - 1 - \ell/2) \]
\[ = b_{2k-2}(P^{\ell}_{n-2}), \quad (15) \]

where the last equality follows from the Sachs theorem. The lemma follows from Eqs. (13)–(15) and the inductive assumption.

The proof of Lemma 2.4 is now complete. □
Similar to Lemma 2.4 we have:

**Lemma 2.5.** Let $\ell = 4r$ and $G \in G(n, \ell)$, but $G \notin C(n, \ell)$. Then $G \prec P_n^\ell$.

**Remark.** In Lemma 2.5, the condition $G \notin C(n, \ell)$ is necessary. For example, for the graph $H$ depicted in Fig. 1 ($\ell = 4, n = 6$), $H \nmid P_6^4$, but $E(H) > E(P_6^4)$.

Combining Lemmas 2.2–2.5 we arrive at:

**Theorem 2.6.** Let $G \in G(n, \ell)$, $n > \ell$. If $G$ has the maximum energy in $G(n, \ell)$, then $G$ is either $P_n^\ell$ or, when $\ell = 4r$, a graph from $C(n, \ell)$.

### 3. Unicyclic bipartite graphs with maximum energy

**Lemma 3.1** ([8]). Let $n = 4k$ or $4k + 1$ or $4k + 2$ or $4k + 3$. Then $P_n \succeq P_4 \cup P_{n-4} \succeq \cdots \succeq P_{2k} \cup P_{n-2k} \succeq P_{2k+1} \cup P_{n-2k-1} \succeq P_{2k-1} \cup P_{n-2k+1} \succeq \cdots \succeq P_3 \cup P_{n-3} \succeq P_1 \cup P_{n-1}$.

**Lemma 3.2.** Let $n \geq 6$. Then $P_n^4 < P_n^6$.

**Proof.** We verify Lemma 3.2 by induction on $n$. By direct calculation we check that the lemma holds for $n = 6$ and $n = 7$. Indeed, the respective characteristic polynomials read:

$$\phi(P_n^4; \lambda) = \lambda^6 - 6\lambda^4 + 6\lambda^2,$$

$$\phi(P_n^6; \lambda) = \lambda^6 - 6\lambda^4 + 9\lambda^2 - 4,$$  

$$\phi(P_7^4; \lambda) = \lambda^7 - 7\lambda^5 + 11\lambda^3 - 2\lambda,$$

$$\phi(P_7^6; \lambda) = \lambda^7 - 7\lambda^5 + 13\lambda^3 - 7\lambda.$$  

Now suppose that $n \geq 8$ and that the statement of the lemma is true for the graphs with $n-1$ and $n-2$ vertices, i.e., that $b_{2k}(P_{n-1}^4) \leq b_{2k}(P_{n-1}^6)$ and $b_{2k}(P_{n-2}^4) \leq b_{2k}(P_{n-2}^6)$. By Lemma 2.3,

$$b_{2k}(P_n^4) = b_{2k}(P_{n-1}^4) + b_{2k-2}(P_{n-2}^4),$$

$$b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6),$$

from which Lemma 3.2 follows straightforwardly. \(\square\)

**Lemma 3.3.** Let $n \geq 6$ and $G \in C(n, 4)$. Then $G \prec P_n^6$.

**Proof.** Again, we use induction on $n$. The lemma holds for $n = 6$ and $n = 7$, which can be checked by means of the table of graphs on six vertices [2] and the data given in Fig. 2 (all graphs from $C(7, 4)$ and their characteristic polynomials).
Suppose that \( n \geq 8 \) and that the statement of the lemma holds for \( n - 1 \) and \( n - 2 \). Let \( uv \) be a pendant edge of \( G \) with pendant vertex \( v \). By Lemma 2.3,

\[
b_{2k}(G) = b_{2k}(G - v) + b_{2k-2}(G - v - u),
\]
\[
b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6).
\]

Since \( G - v - u \) is necessarily acyclic,

\[
b_{2k-2}(G - v - u) = m(G - v - u, k - 1) \leq m(P_{n-2}, k - 1) < b_{2k-2}(P_{n-2}). \quad \square
\]

It is easy to see that

\[
b_{2k}(P_{\ell}^\ell) = \begin{cases} m(P_n^\ell, k) & \text{if } 2k < \ell, \\ m(P_n^\ell, k) - 2m(P_{n-\ell}, k - \ell/2) & \text{if } 2k \geq \ell, \ell = 4r, \\ m(P_n^\ell, k) + 2m(P_{n-\ell}, k - \ell/2) & \text{if } 2k \geq \ell, \ell = 4r + 2. \end{cases}
\]

Thus \( b_{2k}(P_{\ell}^\ell) \leq m(P_{\ell}^\ell, k) + 2 \) when \( n = \ell + 1 \) and \( n = \ell + 2 \).

**Lemma 3.4.** Let \( \ell, \ell \geq 8 \), be even. Then \( P_{\ell+1}^\ell < P_{\ell+1}^6 \).

**Proof.** For \( k \geq 3 \), by Lemmas 2.3 and 3.1,

\[
b_{2k}(P_{\ell+1}^6) = m(P_{\ell+1}^6, k) + 2m(P_{\ell-5}, k - 3)
\]
\[
\geq m(P_{\ell+1}^\ell, k) + m(P_3 \cup P_{\ell-5}, k - 1) + 2m(P_{\ell-5}, k - 3)
\]
\[
\geq m(P_{\ell+1}^\ell, k) + m(P_1 \cup P_{\ell-2}, k - 1) + 2m(P_{\ell-5}, k - 3)
\]
\[
= m(P_{\ell+1}^\ell, k) + 2m(P_{\ell-5}, k - 3)
\]
\[
\geq m(P_{\ell+1}^\ell, k) \pm 2m(P_1, k - \ell/2)
\]
\[
= b_{2k}(P_{\ell+1}^\ell)
\]

where one should note that \( m(P_1, k - \ell/2) \) is equal to zero unless \( k - \ell/2 = 0 \), when it is unity. Similarly, we have \( b_{4d}(P_{\ell+1}^6) = b_{4d}(P_{\ell+1}^\ell). \quad \square
\]

The following two formulas [3,8] are needed in the proof of Lemma 3.5:

\[
m(G_1 \cup G_2, k) = \sum_{i=0}^{k} m(G_1, i)m(G_2, k - i), \tag{16}
\]
\[
m(P_n, k) = m(P_{n-1}, k) + m(P_{n-2}, k - 1). \tag{17}
\]
Lemma 3.5. Let \( \ell, \ell \geq 8 \), be even. Then \( P_{\ell+2}^\ell < P_{\ell+2}^6 \).

Proof. For \( 3 \leq k \leq \ell/2 + 1 \), by repeated use of Eqs. (16), (17) and Lemma 2.3, we get
\[
b_{2k}(P_{\ell+2}^6) = m(P_{\ell+2}^6, k) + 2m(P_{\ell-4}, k - 3) = m(P_{\ell+2}, k) + m(P_4 \cup P_{\ell-4}, k - 1) + 2m(P_{\ell-4}, k - 3) = m(P_{\ell+2}, k) + m(P_{\ell-4}, k - 1) + 3m(P_{\ell-4}, k - 2) + 3m(P_{\ell-4}, k - 3),
\]
\[
b_{2k}(P_{\ell+2}^\ell) = m(P_{\ell+2}^\ell, k) + 2m(P_{\ell-2}, k - \ell/2) \leq m(P_{\ell+2}^\ell, k) + 2 = m(P_{\ell+2}, k) + m(P_2 \cup P_{\ell-2}, k - 1) + 2 = m(P_{\ell+2}, k) + m(P_{\ell-2}, k - 1) + m(P_{\ell-2}, k - 2) + m(P_{\ell-4}, k - 1) + m(P_{\ell-5}, k - 2) + 2m(P_{\ell-4}, k - 2) + m(P_{\ell-4}, k - 3) + m(P_{\ell-5}, k - 3) + 2.
\]
As \( 3 \leq k \leq \ell/2 + 1 \), we have \( 0 \leq k - 3 \leq (\ell - 4)/2 \). If \( k - 3 < (\ell - 4)/2 \), then \( k - 4 < (\ell - 6)/2 \) and \( m(P_{\ell-4}, k - 3) = m(P_{\ell-5}, k - 3) + m(P_{\ell-6}, k - 4) \geq m(P_{\ell-5}, k - 3) \). If \( k - 3 = (\ell - 4)/2 \), then \( m(P_{\ell-4}, k - 3) = 1 > 0 = m(P_{\ell-5}, k - 3) \). Hence, for \( 3 \leq k \leq \ell/2 + 1 \),
\[
m(P_{\ell-4}, k - 2) + 2m(P_{\ell-4}, k - 3) \geq m(P_{\ell-5}, k - 2) + m(P_{\ell-5}, k - 3) + 2.
\]
Therefore
\[
b_{2k}(P_{\ell+2}^6) \geq b_{2k}(P_{\ell+2}^\ell) \quad \text{for all } k \geq 3,
\]
and
\[
b_6(P_{\ell+2}^6) > b_6(P_{\ell+2}^\ell).
\]
Similarly,
\[
b_4(P_{\ell+2}^6) = b_4(P_{\ell+2}^\ell).
\]
Thus \( P_{\ell+2}^\ell < P_{\ell+2}^6 \), and the proof of Lemma 3.5 is completed. \( \square \)

Lemma 3.6. Let \( \ell, \ell \geq 8 \), be even and \( n > \ell \). Then \( P_n^\ell < P_n^6 \).

Proof. We prove the lemma by induction on \( n \). By Lemmas 3.4 and 3.5 the statement is true for \( n = \ell + 1 \) and \( n = \ell + 2 \). Suppose that \( n > \ell + 2 \) and that Lemma 3.6 holds for \( n - 1 \) and \( n - 2 \). By Lemma 2.3,
\[
b_{2k}(P_n^\ell) = b_{2k}(P_{n-1}^\ell) + b_{2k-2}(P_{n-2}^\ell),
\]
\[
b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6). \quad \square
\]
Lemma 3.7. Let $\ell, \ell \geq 8$, be even, $n > \ell$ and $G \in C(n, \ell)$. Then $G \prec P_n^6$.

Proof. We use induction on $n - \ell$. By Lemma 3.4 the statement is true for $n - \ell = 1$. Let $p \geq 2$ and suppose the statement is true for $n - \ell < p$. Consider $n - \ell = p$.

Let $uv$ be a pendant edge of $G$ with pendant vertex $v$. By Lemma 2.3,

$$b_{2k}(G) = b_{2k}(G - v) + b_{2k-2}(G - v - u),$$
$$b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6).$$

Because $G - v - u$ is acyclic,

$$b_{2k-2}(G - v - u) = m(G - v - u, k)$$
$$\leq m(P_{n-2}, k) < b_{2k-2}(P_{n-2}).$$

Summarizing Lemmas 2.2, 3.2, 3.3, 3.6 and 3.7 we arrive at:

Theorem 3.8. Let $G$ be any connected, unicyclic and bipartite graph on $n$ vertices and $G \neq C_n$. Then $E(G) < E(P_n^6)$.

Remark. For $n \geq 8$, neither $C_n \prec P_n^6$ nor $C_n \succ P_n^6$ and therefore $E(P_n^6)$ and $E(C_n)$ cannot be compared by means of Lemma 2.2. To see this, by means of the following identities, which are all from Eq. (9):

$$\phi(P_n^6; \lambda) = \phi(P_n; \lambda) - \phi(P_4; \lambda)\phi(P_{n-6}; \lambda) - 2\phi(P_{n-6}; \lambda),$$
$$\phi(C_n; \lambda) = \phi(P_n; \lambda) - \phi(P_{n-2}; \lambda) - 2,$$
$$\phi(P_{n-2}; \lambda) = \phi(P_4; \lambda)\phi(P_{n-6}; \lambda) - \phi(P_4; \lambda)\phi(P_{n-7}; \lambda),$$
$$\phi(P_{n-6}; \lambda) = \lambda\phi(P_{n-7}; \lambda) - \phi(P_{n-8}; \lambda),$$

we have

$$\phi(C_n; \lambda) = \phi(P_n^6; \lambda) + \phi(C_{n-6}; \lambda) + (\lambda^3 - \lambda)\phi(P_{n-7}; \lambda)$$

(18)

holds for $n \geq 9$. Because expressions for the coefficients of the characteristic polynomials of circuits and paths are well known, from (18) we obtain directly that for even $n$:

$$b_4(C_n) = b_4(P_n^6) + 1$$

implying that $b_4(C_n) > b_4(P_n^6)$, and

$$b_{n-2}(C_n) = b_{n-2}(P_n^6) - \frac{1}{4}(n-6)(n-8)$$

implying that $b_{n-2}(C_n) < b_{n-2}(P_n^6)$ for $n \geq 10$. 


For odd $n$ the situation is similar:

$$b_4(C_n) = b_4(P_n^5) + 1$$

and

$$b_{n-1}(C_n) = b_{n-1}(P_n^5) - (n - 7).$$

Although numerical calculations clearly indicate that for $n \geq 16$ the energy of $P_n^5$ exceeds the energy of $C_n$, at this moment we are not able to offer a formal proof of this inequality. Thus the conjecture of Caporossi et al. remains open.

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