MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **84** (2020) 217-228

ISSN 0340 - 6253

Clar Covering Polynomials with Only Real Zeros*

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(Received January 2, 2020)

Abstract

We present some examples of hexagonal systems whose Clar covering polynomials have only real zeros, and show that all real zeros of Clar covering polynomials are dense in the interval $(-\infty, -1]$.

1 Introduction

Let H be a hexagonal system with at least one Kekulé structure. A *Clar cover* of H is a spanning subgraph of H each (connected) component of which is either a hexagon or an edge. A *resonant pattern* of H is a set of hexagons of a Clar cover of H. The *Clar number* $C(H)$ of H is the maximum number of hexagons in a resonant pattern of H. In 1996, H. Zhang and F. Zhang [22] introduced the concept of Clar covering polynomial $\zeta(H, x)$ of a hexagonal system H:

$$\zeta(H, x) = \sum_{k=0}^{C(H)} c(H, k) x^k,$$

where $c(H, k)$ denotes the number of Clar covers of H having precisely k hexagons. Such a polynomial is also called the *Zhang-Zhang polynomial* in the literature [9, 11]. For

*This work was partially supported by NSFC of China (No. 11771065).

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example, let C and T be the coronene and the triphenylene as shown in Figure 1. Then $\zeta(C,x) = 2x^3 + 14x^2 + 30x + 19$ and $\zeta(T,x) = x^3 + 6x^2 + 13x + 9$.

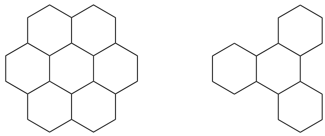

Figure 1. Coronene C and triphenylene T

The knowledge of Clar covering polynomials yield immediately a number of important topological invariants. For example, the first term $c(H, C(H))$ and the constant term $c(H, 0)$ count the numbers of the Clar structures and the Kekulé structures of H respectively. Zhang and Zhang [23, Conjecture 8] conjectured that the Clar covering polynomial of any hexagonal system has unimodal coefficients. A sequence $a_0, a_1, \ldots, a_n$ of nonnegative numbers is *unimodal* if

$$a_0 \leq a_1 \leq \cdots \leq a_m \geq a_{m+1} \geq \cdots \geq a_n$$

for some m, and *log-concave* if

$$a_{k-1}a_{k+1} \leq a_k^2, \qquad k = 1, 2, \ldots, n-1.$$

Clearly, a log-concave sequence of positive numbers is unimodal. A classical approach for attacking the unimodality and log-concavity problem is to use the Newton inequality: If the real polynomial $f(x) = a_0 + a_1x + \cdots + a_nx^n$ has only real zeros, then

$$a_k^2 \geq a_{k-1}a_{k+1}\frac{(k+1)(n-k+1)}{k(n-k)}, \qquad k = 1, 2, \ldots, n-1.$$

In particular, if all coefficients a_k are nonnegative, then the sequence of coefficients is log-concave and unimodal [12, p.104]. So it is natural to ask for which hexagonal systems the Clar covering polynomials have only real zeros.

A concept closely related to the Clar covering polynomial is the sextet polynomial. The *sextet polynomial* of a hexagonal system H is defined as

$$\sigma(H, x) = \sum_{k=0}^{C(H)} s(H, k)x^k,$$

where $s(H, k)$ denotes the number of resonant patterns of H having precisely k hexagons and $s(H, 0) = 1$ if H has a Kekulé structure. A hexagonal system H is called *thin* if H has no coronene C as its nice subgraph (a subgraph C of H is called *nice* if either $H - C$ has a perfect matching or $H - C$ is empty). It is known [23] that $\zeta(H, x) = \sigma(H, x+1)$ if H is a thin hexagonal system. Gutman [7] showed that the sextet polynomial of a hexagonal chain is precisely the matching polynomial of the corresponding Gutman tree. Gutman [8] also showed that the sextet polynomial of a resonant hexagonal system coincides with the independence polynomial of the corresponding Clar graph (see [13] for more information). On the other hand, Gutman and Godsil [6] showed that the matching polynomial of a graph has only real zeros. Chudnovsky and Seymour [5] showed that the independence polynomial of a clawfree graph has only real zeros. As a result, many Clar covering polynomials have only real zeros.

Zhang et al. [21, Theorem 2.8] showed that if H is a Kekuléan hexagonal system, then $\zeta(H, x) = C(R(H), x)$, where $R(H)$ is the resonance graph of H and $C(G, x)$ is the cube polynomial of a median graph G. Brešar et al. [2, Theorem 5.1] showed that every cube polynomial has one real zero in the interval $[-2, -1)$, and so has every Clar covering polynomial. They also showed that there is no cube zeros in the interval $[-1, +\infty)$ and there exists arbitrarily small negative real cube zeros [2, Corollary 3.2 and Proposition 5.2]. Zhang et al. [21, Theorem 4.11] showed that every cube polynomial can be expressed in the power of $(x + 1)$ with nonnegative coefficients.

In this paper we present some non-trivial examples of hexagonal systems whose Clar covering polynomials have only real zeros. We also show that all real zeros of Clar covering polynomials are dense in the interval $(-\infty, -1]$.

Throughout the paper, all terms used but not defined can be found in [10].

2 Clar covering polynomials with only real zeros

In this section we show that Clar covering polynomials of some hexagonal systems have only real zeros by means of various approaches.

2.1 The phenanthrene chain B_n

Let B_n be the hexagonal system as shown in Figure 2. Then

$$\sigma(B_n, x) = 1 + 3nx + n(2n-1)x^2 + \frac{n(n-1)(2n-1)}{6}x^3$$

(see [16] for instance). Clearly, B_n is thin, and so $\zeta(B_n, x) = \sigma(B_n, x + 1)$.

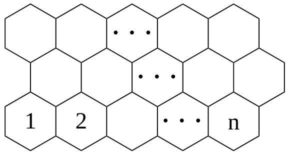

Figure 2. B_n

It is easy to check that $\sigma(B_n, -3/n) > 0$ and $\sigma(B_n, -1/n) < 0$. Hence all real zeros of $\sigma(B_n, x)$ are located in $(-\infty, -3/n), (-3/n, -1/n)$ and $(-1/n, +\infty)$ respectively. Thus $\sigma(B_n, x)$ has only real zeros. This result can also be followed from the following folklore result (see [14] for instance).

Lemma 2.1. *Let* $f(x) = \sum_{k=0}^{n} a_k x^k$ *be a polynomial with positive coefficients. If*

$$a_k^2 > 4a_{k-1}a_{k+1}$$

for $k = 1, 2, \ldots, n-1$*, then zeros of* $f(x)$ *are real and distinct.*

On the other hand, we have $\zeta(B_n, x) = \sigma(B_n, x+1)$ since B_n is obviously a thin hexagonal system. We conclude the following result.

Proposition 2.2. *The Clar covering polynomials* $\zeta(B_n, x)$ *have only real zeros.*

2.2 The multiple linear hexagonal chain $P(m, n)$

Let $P(m, n)$ be the hexagonal system as shown in Figure 3. Gutman and Borovićanin [9] showed that the Clar covering polynomial

$$\zeta(P(m,n), x) = \sum_{k=0}^{\min\{m,n\}} \binom{m}{k} \binom{n+m-k}{m} x^k,$$

which can be expressed as

$$\zeta(P(m,n), x) = \sum_{k=0}^{\min\{m,n\}} \binom{m}{k} \binom{n}{k} (x+1)^k$$

(see [4] for instance).

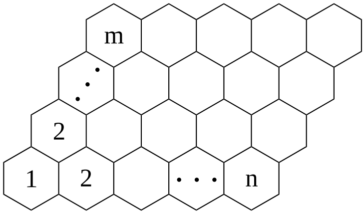

Figure 3. $P(m, n)$

Recall the following classical result (see [19] for instance).

Lemma 2.3 (Malo, 1895)**.** *Suppose that* $f(x) = \sum_{k=0}^{n} a_k x^k$ *and* $g(x) = \sum_{k=0}^{m} b_k x^k$ *are two polynomials with only real zeros and all* b_i *have the same sign. Then the polynomial*

$$(f \circ g)(x) = \sum_{i=0}^{\min\{n,m\}} a_k b_k x^k$$

has only real zeros.

It follows immediately that the polynomial

$$\sum_{k=0}^{\min\{m,n\}} \binom{m}{k}\binom{n}{k} x^k = (x+1)^m \circ (x+1)^n$$

has only real zeros. Thus we obtain the following result.

Proposition 2.4. *The Clar covering polynomials* $\zeta(P(m, n), x)$ *have only real zeros.*

2.3 The hexagonal system U_n

Since the Clar covering polynomials of hexagonal systems often satisfy certain recurrence relations, the following criterion, which is a special case of [15, Theorem 2.3], will be very useful.

Lemma 2.5. *Let* $(f_n(x))_{n\geq 0}$ *be a sequence of polynomials of positive coefficients with* $\deg f_0 = 0$ *and* $\deg f_{n-1} \leq \deg f_n \leq \deg f_{n-1} + 1$. *Suppose that*

$$f_n(x) = b(x) f_{n-1}(x) + a(x) f_{n-2}(x), \quad n = 2, 3, \ldots,$$

where $a(x)$ *and* $b(x)$ *are real polynomials. If* $a(x) \leq 0$ *for* $x \leq 0$, *then all* $f_n(x)$ *have only real zeros.*

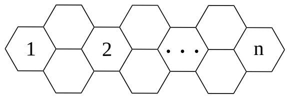

Figure 4. U_n

Let U_n be the hexagonal system as shown in Figure 4. Then

$$\sigma(U_n, x) = (1 + 2x)\sigma(U_{n-1}, x) + x(1 - x)\sigma(U_{n-2}, x)$$

with $\sigma(U_0, x) = 1$ and $\sigma(U_1, x) = 1 + x$ (see [17] for instance). It follows immediately from Lemma 2.5 that $\sigma(U_n, x)$ has only real zeros. Now $\zeta(U_n, x) = \sigma(U_n, x + 1)$ since U_n are thin hexagonal systems. Hence we have the following result.

Proposition 2.6. *The Clar covering polynomials $\zeta(U_n, x)$ have only real zeros.*

2.4 The pyrene chain P_n

The following result is also very useful in studying the location of a polynomial sequence satisfying the recurrence relation. Denote by $\Re(z)$ and $\Im(z)$ the real and imaginary part of a complex number z, respectively.

Lemma 2.7 ([18, Theorem 1]). *Let $(f_n(z))_{n\geq 0}$ be a sequence of polynomials whose generating function is*

$$\sum_{n\geq 0} f_n(z)t^n = \frac{1}{1 + B(z)t + A(z)t^2}$$

where $A(z)$ and $B(z)$ are two complex polynomials. Then the zeros of $f_n(z)$ which satisfy $A(z) \neq 0$ lie on the curve $\mathcal{C}$ defined by

$$\begin{cases} \Im\left[\frac{B^2(z)}{A(z)}\right] = 0 \\ 0 \leq \Re\left[\frac{B^2(z)}{A(z)}\right] \leq 4, \end{cases}$$

and are dense there as $n \to +\infty$.

Corollary 2.8. *Let $(f_n(z))_{n\geq 0}$ be a sequence of polynomials of real coefficients satisfying*

$$f_n(z) = c(z)f_{n-1}(z) - z^2 f_{n-2}(z) \qquad (1)$$

with $f_0(z) = 1$ and $f_1(z) = c(z)$. Then the nonzero zeros of $f_n(z)$ lie on the curve $\mathcal{C}$ defined by

$$\begin{cases} \Im\left[\frac{c(z)}{z}\right] = 0 \\ -2 \leq \Re\left[\frac{c(z)}{z}\right] \leq 2, \end{cases} \qquad (2)$$

and are dense there as $n \to +\infty$.

Proof. Note first that (1) implies

$$\sum_{n\geq 0} f_n(z)t^n = \frac{1}{1-c(z)t+z^2t^2}.$$

Now let $\Re\left[\frac{c(z)}{z}\right] = u$ and $\Im\left[\frac{c(z)}{z}\right] = v$. Then

$$\frac{c^2(z)}{z^2} = (u+vi)^2 = (u^2-v^2)+2uvi.$$

By Lemma 2.7, the curve $\mathcal{C}$ is decided by $v=0$ and $u^2 \leq 4$, as required. ∎

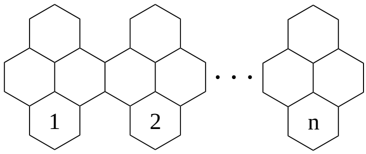

Figure 5. P_n

Let P_n be the hexagonal systems as shown in Figure 5. Then

$$\sigma(P_n,x) = (x^2+4x+1)\sigma(P_{n-1},x) - x^2\sigma(P_{n-2},x)$$

with $\sigma(P_0,x)=1$ and $\sigma(P_1,x)=x^2+4x+1$ (see [16] for instance). Now $c(x)=x^2+4x+1$, which has two real zeros. Assume that $z_0=a+bi$ is a non-real zeros of a certain $\sigma(P_n,x)$. Then

$$\frac{c(z_0)}{z_0} = \left(a+4+\frac{a}{a^2+b^2}\right)+\left(1-\frac{1}{a^2+b^2}\right)bi.$$

By the equality in (2), we have $a^2+b^2=1$, and so $|a|<1$. It follows that

$$\left|a+4+\frac{a}{a^2+b^2}\right| = |2a+4| \geq 4-2|a| > 2,$$

a contradiction to the inequality in (2). Thus $\sigma(P_n,x)$ have only real zeros. Since the hexagonal systems P_n are thin, we have the following result.

Proposition 2.9. *The Clar covering polynomials $\zeta(P_n,x)$ have only real zeros.*

2.5 The hexagonal system $L(n)$

Let $L(n)$ be the hexagonal systems as shown in Figure 6.

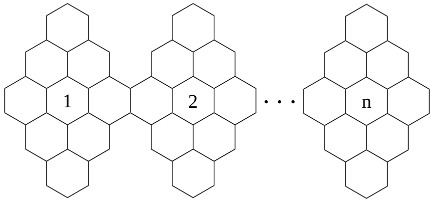

Figure 6. $L(n)$

Zhang et al. [20] gave the explicit expression of the sextet polynomial of $L(n)$ by means of the transfer-matrix method:

$$\sigma(L(n),x)=\frac{\lambda_1^{n+1}-\lambda_2^{n+1}}{\lambda_1-\lambda_2}, \tag{3}$$

where

$$\lambda_{1,2}=\frac{x^3+9x^2+9x+1\pm\sqrt{x^6+18x^5+99x^4+164x^3+95x^2+18x+1}}{2}.$$

We next show that $\sigma(L(n),x)$ have only real zeros. We do this only for n even since the case is similar for n odd. Recall that the identity

$$\lambda_1^{2n+1}-\lambda_2^{2n+1}=(\lambda_1-\lambda_2)\prod_{k=1}^{n}\left[(\lambda_1+\lambda_2)^2-4\lambda_1\lambda_2\cos^2\frac{k\pi}{2n+1}\right].$$

Now $\lambda_1+\lambda_2=x^3+9x^2+9x+1$ and $\lambda_1\lambda_2=x^2$. Hence

$$\begin{aligned}\sigma(L(n),x) &= \prod_{k=1}^{n}\left[(x^3+9x^2+9x+1)^2-4x^2\cos^2\frac{k\pi}{2n+1}\right]\\ &= \prod_{k=1}^{2n}\left(x^3+9x^2+9x+1-2x\cos\frac{k\pi}{2n+1}\right).\end{aligned}$$

It follows from Lemma 2.1 that $x^3+9x^2+9x+1-2cx$ has only real zeros for $-1<c<1$, so does $\sigma(L(n),x)$. Note that $L(n)$ are thin hexagonal systems. Hence we have the following result.

Proposition 2.10. *The Clar covering polynomials $\zeta(L(n),x)$ have only real zeros.*

3 Distribution of real Clar covering zeros

It is known [21, Corollary 4.7] that there is no Clar covering zeros in the interval $[-1,+\infty)$. In this section we show that real Clar covering zeros are dense in the interval $(-\infty,-1]$. We need the following lemma.

Let $(f_n(x))_{n\geq 0}$ be a sequence of complex polynomials. We say that the complex number x is a *limit of zeros* of the sequence $(f_n(x))_{n\geq 0}$ if there is a sequence $(z_n)_{n\geq 0}$ such that $f_n(z_n) = 0$ and $z_n \to x$ as $n \to +\infty$. Suppose now that $(f_n(x))_{n\geq 0}$ is a sequence of polynomials satisfying the recursion

$$f_{n+k}(x) = -\sum_{j=1}^{k} c_j(x) f_{n+k-j}(x)$$

where $c_j(x)$ are polynomials in x. Let $\lambda_j(x)$ be all zeros of the associated characteristic equation $\lambda^k + \sum_{j=1}^{k} c_j(x)\lambda^{k-j} = 0$. It is well known that if $\lambda_j(x)$ are distinct, then

$$f_n(x) = \sum_{j=1}^{k} \alpha_j(x)\lambda_j^n(x), \tag{4}$$

where $\alpha_j(x)$ are determined from the initial conditions.

Lemma 3.1 ([1, Theorem]). *Under the non-degeneracy requirements that in* (4) *no* $\alpha_j(x)$ *is identically zero and that for no pair* $i \neq j$ *is* $\lambda_i(x) \equiv \omega\lambda_j(x)$ *for some* $\omega \in \mathbb{C}$ *of unit modulus, then* x *is a limit of zeros of* $(f_n(x))_{n\geq 0}$ *if and only if either*

(i) *two or more of the* $\lambda_i(x)$ *are of equal modulus, and strictly greater (in modulus) than the others; or*

(ii) *for some* j, $\lambda_j(x)$ *has modulus strictly greater than all the other* $\lambda_i(x)$ *have, and* $\alpha_j(x) = 0$.

Corollary 3.2. *Let* $(f_n(x))_{n\geq 0}$ *be a sequence of real polynomials satisfying the recurrence relation*

$$f_n(x) = b(x)f_{n-1}(x) + a(x)f_{n-2}(x), \quad n = 2, 3, \ldots,$$

where $a(x), b(x) \in \mathbb{R}[x]$, $b^2(x) + 4a(x)$ *is not identically zero. Suppose that* $f_n(x)/f_{n-1}(x)$ *are not identical for all* n. *If all* $f_n(x)$ *have only real zeros, then these zeros are dense on the set*

$$I = \{x \in \mathbb{R} : b^2(x) + 4a(x) \leq 0\}.$$

For $m \geq 2$, let $L(m, n)$ be the hexagonal chains shown as in Figure 7. Then

$$\zeta(L(m,n),x) = [(m-2)x + (m-1)]\zeta(L(m,n-1),x) + (x+1)\zeta(L(m,n-2),x) \tag{5}$$

with $\zeta(L(m,0),x) = 1$ and $\zeta(L(m,1),x) = mx + m + 1$ (see [3,22] for instance). We next discuss the location of zeros of all $\zeta(L(m,n),x)$.

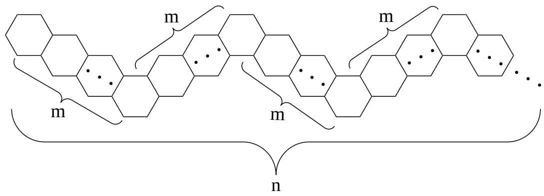

Figure 7. $L(m,n)$

Consider first the case $m = 2$. In this case,

$$\zeta(L(2,n),x) = \zeta(L(2,n-1),x) + (x+1)\zeta(L(2,n-2),x)$$

with $\zeta(L(2,0),x) = 1$ and $\zeta(L(2,1),x) = 2x+3$. It follows from Corollary 3.2 that zeros of all $\zeta(L(2,n),x)$ are dense in the set $\{x \in \mathbb{R} : 1 + 4(x+1) \leq 0\}$, i.e., $x \in (-\infty, -5/4]$.

We next consider the case $m \geq 3$. Then zeros of $\zeta(L(m,n),x)$ are dense in the set

$$\{x \in \mathbb{R} : (m-2)^2(x+1)^2 + 2m(x+1) + 1 \leq 0\},$$

i.e., $x \in I_m = [a_m, b_m]$, where

$$a_m = -\frac{1}{(\sqrt{m-1}-1)^2} - 1, \quad b_m = -\frac{1}{(\sqrt{m-1}+1)^2} - 1. \tag{6}$$

Clearly, $(a_m), (b_m)$ are increasing sequences and $a_{m+1} < b_m$ for $m \geq 3$. Hence $I_m \cap I_{m+1} \neq \emptyset$. Also, $a_3 = -2(2+\sqrt{2})$ and $b_m \to -1$ when $m \to +\infty$. Thus zeros of $\zeta(L(m,n),x)$ for $m \geq 3$ are dense in the interval $[-2(2+\sqrt{2}), -1]$.

Since $-2(2+\sqrt{2}) < -5/4$, we conclude that zeros of $\zeta(L(m,n),x)$ for $m \geq 2$ are dense in the interval $(-\infty, -1]$. Thus we have the following result.

Theorem 3.3. *Real Clar covering zeros are dense in the interval* $(-\infty, -1]$.

4 Further work

The Clar covering polynomial of a hexagonal system may have non-real zeros. For example, the Clar covering polynomial of the triphenylene T is

$$\zeta(T,x) = x^3 + 6x^2 + 13x + 9,$$

whose three zeros are

$$x_1 \approx -1.32, \quad x_2 \approx -2.34 + 1.16i, \quad x_3 \approx -2.34 - 1.16i.$$

By checking small hexagonal systems, we found that the real part of every zero of Clar covering polynomials is less than -1. It is possible that all Clar covering polynomials have such properties.

H. Zhang and F. Zhang [23, Conjecture 8] conjectured that the Clar covering polynomial of a hexagonal system has unimodal coefficients. Numerical results suggest the following stronger conjecture.

Conjecture 4.1. *The Clar covering polynomial of a hexagonal system has log-concave coefficients.*

Acknowledgment: The authors thank the anonymous referee for valuable comments and suggestions.

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