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New Approaches for the Real and Complex Integral Formulas of the Energy of a Polynomial

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Abstract

The energy of a graph was first defined in 1977. In 2010 (but also earlier) this concept was generalized to the energy of any complex polynomial. In this paper, we adopt new approaches to prove both the complex form and real form of the Coulson integral formulas for the energy of a complex polynomial. For the complex form, we use an approach which does not use the contour integration and the Cauchy residue theorem. For the real form, we use an approach which can completely avoid using the logarithm of a complex function. We also obtain the following new formula for the energy of an arbitrary monic complex polynomial $\phi(z)$:

$$\mathbb{E}(\phi) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log\left[p^2(x) + q^2(x)\right] dx + \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2}\, arctg \frac{q(x)}{p(x)}\, dx$$

where the real polynomials $p(x)$ and $q(x)$ are the real and imaginary parts of $g(-ix)$, while $g(t)$ is the so called "reverse polynomial" of $\phi(t)$. Finally, we give some applications of these results to the energies of digraphs.

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1 Introduction

The energy of a graph G was conceived in the 1970s by one of the present authors [4] (see also [5]). However, the chemical aspects of this concept can be traced back until the 1940s [1]. The energy of a graph G is defined as the sum of the absolute values of the eigenvalues (of the adjacency matrix) of G. Since then, this definition has various generalizations. The most recent generalization was in [11] where the energy of any complex polynomial was defined in such a way that the energy of a graph, or a digraph, is just the energy of its characteristic polynomial.

In a much earlier work [7], one of the present authors considered a somewhat related problem. Among other things, in [7] was proven that if $A(x)$ and $B(x)$ are two monic (but otherwise arbitrary) polynomials of equal degree n, and if $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ are the zeros of $A(x)$ and $B(x)$, respectively, then

$$\frac{1}{\pi}\, p.v. \int_{-\infty}^{+\infty} \log \frac{A(ix)}{B(ix)}\, dx = \sum_{j=1}^{n} \Big[|Re(a_j)| - |Re(b_j)| \Big] \, .$$

This formula holds provided $a_1 + \cdots + a_n = b_1 + \cdots + b_n$.

The present paper can be viewed as the elaboration and analysis of the concept of the energy of an arbitrary polynomial, at a rigorous mathematical level.

Definition 1.1. [11] Let

$$\phi(z) = \sum_{k=0}^{n} a_k\, z^{n-k} = (z - z_1)(z - z_2) \cdots (z - z_n)$$

be a monic complex polynomial of degree n. Then its (complex) energy $\mathbb{E}(\phi)$ is defined as:

$$\mathbb{E}(\phi) = \sum_{k=1}^{n} sgn(\mathrm{Re}(z_k))\, z_k \tag{1.1}$$

where $sgn(a)$ of a real number a is defined to be 1, 0, or -1, according to $a > 0$, $a = 0$, or $a < 0$.

The real energy $\mathbb{E}_{re}(\phi)$ of $\phi(z)$ is defined to be the real part of the energy $\mathbb{E}(\phi)$. Namely [11],

$$\mathbb{E}_{re}(\phi) = \mathrm{Re}(\mathbb{E}(\phi)) \, .$$

It was pointed out in [11] that (1.1) can be rewritten as

$$\mathbb{E}(\phi) = \sum_{\mathrm{Re}(z_k)>0} z_k - \sum_{\mathrm{Re}(z_k)<0} z_k \tag{1.2}$$

and

$$\mathbb{E}_{re}(\phi) = \sum_{k=1}^{n} |\operatorname{Re}(z_k)| \ . \tag{1.3}$$

In the special case where $\phi(z)$ is a real polynomial (but possibly has complex roots), then its non-real roots occur in pairs (counting the multiplicities). In this case

$$\sum_{\operatorname{Re}(z_k)>0} \operatorname{Im}(z_k) = 0 = \sum_{\operatorname{Re}(z_k)<0} \operatorname{Im}(z_k) \ .$$

Thus from (1.2) we have $\operatorname{Im}(\mathbb{E}(\phi)) = 0$. So in this case one has [11]

$$\mathbb{E}(\phi) = \mathbb{E}_{re}(\phi) = \sum_{k=1}^{n} |\operatorname{Re}(z_k)| \ . \tag{1.4}$$

If we further assume that all the roots of $\phi(z)$ are real (for example, $\phi(z)$ is the characteristic polynomial of a symmetric real matrix, or of a graph), then $\operatorname{Re}(z_k) = z_k \ (k = 1, \ldots, n)$. Then from (1.4) we further have (see [11])

$$\mathbb{E}(\phi) = \mathbb{E}_{re}(\phi) = \sum_{k=1}^{n} |z_k| \ .$$

This coincides with the original definition of the energy of a (undirected) graph, or a symmetric real matrix.

Let $\phi(z) = \phi_G(z)$ be the characteristic polynomial of a graph G. Coulson [1] obtained the following integral formula for the energy of the graph G:

$$\mathbb{E}(G) = \mathbb{E}(\phi) = \frac{1}{\pi} \ p.v. \int_{-\infty}^{+\infty} \left[n - \frac{iy\,\phi'(iy)}{\phi(iy)} \right] dy \tag{1.5}$$

where the principal value ($p.v.$) of the integral $\int_{-\infty}^{+\infty}$ means $\lim_{M\to+\infty} \int_{-M}^{M}$. Note that if $\phi(z)$ has purely imaginary roots $ib_1, \ldots, ib_r$ (with $b_1 < \cdots < b_r$), then the $p.v.$ of the integral in (1.5) will mean:

$$\lim_{\substack{M\to+\infty \\ \varepsilon_j\to 0(j=1,\cdots,r)}} \int_{-M}^{b_1-\varepsilon_1} + \sum_{j=1}^{r-1} \int_{b_j+\varepsilon_j}^{b_{j+1}-\varepsilon_{j+1}} + \int_{b_r+\varepsilon_r}^{M} \ .$$

In [10] and [11], Mateljević et al. proved that the integral formula (1.5) also holds for any complex polynomial $\phi(z)$, by using partial fraction decomposition, the Cauchy residue formula, the Jordan lemma and complex integration along semicircle.

For convenience, we call (1.5) the *complex form of the Coulson integral formula* (or simply complex integral formula) for the energy of a polynomial.

In [11], Mateljević et al. also gave a real integral formula for the real energy of a polynomial.

In this paper we give new proofs for both the complex integral formula and the real integral formula for the energy, and real energy, of a polynomial.

In §2, we give a new proof of the complex integral formula without using the contour integration, the Cauchy residue formula and the Jordan lemma.

In §3, we outline an approach that completely avoids the use of the logarithm of a complex function when proving the real form of the integral formula for the real energy of a complex polynomial. There we also obtain the following new formula for the energy of an arbitrary monic complex polynomial $\phi(z)$:

$$\mathbb{E}(\phi) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log\left[p^2(x) + q^2(x)\right] dx + \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2}\, arctg \frac{q(x)}{p(x)}\, dx$$

where the real polynomials $p(x)$ and $q(x)$ are the real and imaginary parts of $g(-ix)$, while $g(t)$ is the so called "reverse polynomial" of $\phi(t)$.

Note that the complex function $log\ z$ is a multi-valued function. We usually need to take a specific branch of $log\ z$ to study it. This will sometimes cause difficulties. For example, $log\ (ab) = log\ a + log\ b$ is not always true for complex numbers a and b, when $0 \leq arg(a) < 2\pi$, $0 \leq arg(b) < 2\pi$, but $arg(a) + arg(b) > 2\pi$ (as was pointed out in [11]).

2 The complex Coulson integral formula

In this section, we give a new proof of the following complex form (2.1) of Coulson integral formula for the energy of an arbitrary complex polynomial $\phi(z)$, without using contour integration, or the Cauchy residue formula for the integration of complex variable functions. A simplified consideration along the same lines was reported already in the paper [4], and eventually reproduced on pp. 55–56 of the book [3].

What first needs to be noted is that formula (2.1) is a proper generalization of formula (1.5):

$$\mathbb{E}(\phi) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{iy\, \phi'(iy)}{\phi(iy)} \right] dy\ . \tag{2.1}$$

Recall that $sgn(a)$ denotes the sign of a real number a.

Lemma 2.1. *For any real numbers a and b,*

$$\int_{-\infty}^{+\infty} \frac{a}{(x-b)^2+a^2}\,dx = \pi \cdot sgn(a)\ .$$

Proof. The result holds obviously if $a=0$. So we now assume that $a \neq 0$.

Using $a = |a| sgn(a)$, and taking $y = (x-b)/|a|$, we have

$$\int_{-\infty}^{+\infty} \frac{a}{(x-b)^2+a^2}\,dx = sgn(a) \int_{-\infty}^{+\infty} \frac{1}{\left(\frac{x-b}{|a|}\right)^2+1}\, d\left(\frac{x-b}{|a|}\right)$$

$$= \ sgn(a) \int_{-\infty}^{+\infty} \frac{1}{y^2+1}\,dy = sgn(a)\ arctg\ y \Big|_{-\infty}^{+\infty} = \pi \cdot sgn(a)\ .$$

□

Lemma 2.2. *For any real numbers a and b,*

$$\lim_{M\to+\infty} \int_{-M}^{M} \frac{x-b}{(x-b)^2+a^2}\,dx = 0\ .$$

Proof. **Case 1:** $a=0$. Then the integral should be understood as the following principal value:

$$\lim_{\substack{M\to+\infty\\ \varepsilon\to 0}} \left[\int_{-M}^{b-\varepsilon} \frac{1}{x-b}\,dx + \int_{b+\varepsilon}^{M} \frac{1}{x-b}\,dx\right] \ = \ \lim_{\substack{M\to+\infty\\ \varepsilon\to 0}} \left[\log|x-b| \Big|_{-M}^{b-\varepsilon} + \log|x-b| \Big|_{b+\varepsilon}^{M}\right]$$

$$= \ \lim_{\substack{M\to+\infty\\ \varepsilon\to 0}} \log\left|\frac{M-b}{M+b}\right| = 0\ .$$

Case 2: $a \neq 0$. Then we have

$$\int_{-M}^{M} \frac{x-b}{(x-b)^2+a^2}\,dx \ = \ \frac{1}{2}\log[(x-b)^2+a^2]\Big|_{-M}^{M}$$

$$= \ \frac{1}{2}\log\left[\frac{(M-b)^2+a^2}{(M+b)^2+a^2}\right] \to 0 \qquad (\text{when } M\to+\infty)\ .$$

□

Theorem 2.1. *For any complex polynomial $\phi(z) = (z-z_1)\cdots(z-z_n)$, the complex Coulson integral formula (2.1) holds.*

Proof. Let $z_k = a_k + b_k i$ ($a_k,\ b_k$ are real numbers, $k = 1, \ldots, n$) and let

$$f(z) = n - \frac{z\,\phi'(z)}{\phi(z)}\ .$$

Then

$$f(z) = n - \sum_{k=1}^{n} \frac{z}{z - z_k} = \sum_{k=1}^{n} \frac{z_k}{z_k - z}$$

implying

$$\frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{iy\phi'(iy)}{\phi(iy)} \right] dy = \frac{1}{\pi} \int_{-\infty}^{+\infty} f(iy)\, dy = \frac{1}{\pi} \sum_{k=1}^{n} \int_{-\infty}^{+\infty} \frac{z_k}{z_k - iy}\, dy\ . \tag{2.2}$$

By using Lemmas 2.1 and 2.2 we get

$$\begin{aligned}
\int_{-\infty}^{+\infty} \frac{z_k}{z_k - iy}\, dy &= \int_{-\infty}^{+\infty} \frac{a_k + b_k i}{a_k - (y - b_k) i}\, dy \\
&= \int_{-\infty}^{+\infty} \frac{a_k^2 - b_k(y - b_k) + [a_k(y - b_k) + a_k b_k] i}{(y - b_k)^2 + a_k^2}\, dy \\
&= \pi a_k \cdot sgn(a_k) + \pi b_k \cdot sgn(a_k) i = \pi \cdot sgn(a_k)(a_k + b_k i) \\
&= \pi \cdot sgn(a_k)\, z_k\ . \qquad (2.3)
\end{aligned}$$

Substituting (2.3) into (2.2), we arrive at

$$\frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{iy\phi'(iy)}{\phi(iy)} \right] dy = \frac{1}{\pi} \sum_{k=1}^{n} \pi \cdot sgn(a_k)\, z_k = \sum_{k=1}^{n} sgn(\mathrm{Re}(z_k))\, z_k = \mathbb{E}(\phi)\ .$$

□

3 The real integral formulas

In this section, we put forward an approach that can completely avoid using the logarithm of a complex function to prove the real form of the integral formula for the real energy of a complex polynomial. We also obtain the following new formula for the energy of an arbitrary monic complex polynomial $\phi(z)$:

$$\mathbb{E}(\phi) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log\left[p^2(x) + q^2(x)\right] dx + \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2}\ arctg \frac{q(x)}{p(x)}\, dx$$

where the real polynomials $p(x)$ and $q(x)$ are the real and imaginary parts of $g(-ix)$, while $g(t)$ is the so called "reverse polynomial" of $\phi(t)$.

Now let $\phi(z) = \sum_{k=0}^{n} a_k\, z^{n-k}$ be a complex polynomial with $a_0 = 1$ and $a_k = b_k + c_k\, i$, where b_k and c_k are real numbers $(k = 0, 1, \cdots, n)$. Also we write $f(z) = n - z\,\phi'(z)/\phi(z)$. Then we have:

$$
\begin{aligned}
f(z) &= n - \frac{z\phi'(z)}{\phi(z)} = n - \frac{\sum\limits_{k=0}^{n} (n-k)\, a_k\, z^{n-k}}{\sum\limits_{k=0}^{n} a_k\, z^{n-k}} \\
&= \frac{\sum\limits_{k=0}^{n} k\, a_k\, z^{n-k}}{\sum\limits_{k=0}^{n} a_k\, z^{n-k}} = \frac{\sum\limits_{k=0}^{n} k\, a_k\, (1/z)^k}{\sum\limits_{k=0}^{n} a_k\, (1/z)^k} . \qquad (3.1)
\end{aligned}
$$

Let $g(t) = \sum_{k=0}^{n} a_k\, t^k$ be the polynomial obtained from $\phi(t)$ by reversing the order of the coefficients of $\phi(t)$. For convenience, we call $g(t)$ the "reverse polynomial" of $\phi(t)$. Then from (3.1) we have:

$$
f(1/t) = \frac{\sum\limits_{k=0}^{n} k\, a_k\, t^k}{\sum\limits_{k=0}^{n} a_k\, t^k} = \frac{t\, g'(t)}{g(t)} .
$$

By changing the variable $t = 1/x$ in the integration, writing $D_M = (-\infty, -\frac{1}{M}) \cup (\frac{1}{M}, +\infty)$, and using the complex integral formula (2.1), we have

$$
\begin{aligned}
\int_{-M}^{M} f(it)\, dt &= \int_{-\infty}^{-1/M} f(i/x)\, \frac{dx}{x^2} + \int_{1/M}^{+\infty} f(i/x)\, \frac{dx}{x^2} = \int_{D_M} \frac{(x/i)\, g'(x/i)}{g(x/i)\, x^2}\, dx \\
&= \int_{D_M} \frac{(g(x/i))'}{x\, g(x/i)}\, dx \longrightarrow \pi\, \mathbb{E}(\phi) \qquad (\text{when } M \to +\infty) . \qquad (3.2)
\end{aligned}
$$

Now we write

$$
g(x/i) = g(-ix) = p(x) + i\, q(x)
$$

recalling that $p(x)$ and $q(x)$ are real polynomials. Then $(g(x/i))' = p'(x) + i\, q'(x)$. Thus the real part of the integrand in (3.2) is:

$$
\begin{aligned}
\mathrm{Re}\left[\frac{(g(x/i))'}{x\, g(x/i)}\right] &= \mathrm{Re}\left(\frac{p'(x) + iq'(x)}{x[p(x) + iq(x)]}\right) = \frac{p(x)\, p'(x) + q(x)\, q'(x)}{x(p^2(x) + q^2(x))} \\
&= \left[\frac{1}{2x} \log\left[p^2(x) + q^2(x)\right]\right]' + \frac{1}{2x^2} \log\left[p^2(x) + q^2(x)\right] . \qquad (3.3)
\end{aligned}
$$

Here the function inside log is a real function.

Since $g(t) = \sum_{k=0}^{n} a_k\, t^k = \sum_{k=0}^{n} b_k\, t^k + (\sum_{k=0}^{n} c_k\, t^k)\, i$, we have

$$g(-ix) = \sum_{k=0}^{n} b_k(-ix)^k + \left(\sum_{k=0}^{n} c_k(-ix)^k\right) i \ .$$

From this and the assumption $a_0 = b_0 + c_0\, i = 1$ we obtain

$$p(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, b_{2k}\, x^{2k} + \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} (-1)^k\, c_{2k+1}\, x^{2k+1} = 1 + c_1\, x + \cdots \tag{3.4}$$

$$q(x) = \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} (-1)^{k+1}\, b_{2k+1}\, x^{2k+1} + \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, c_{2k}\, x^{2k} = -b_1\, x + \cdots \tag{3.5}$$

Thus there exists some real polynomial $h(x)$, such that

$$p^2(x) + q^2(x) = 1 + 2c_1\, x + x^2\, h(x) \ .$$

Then $\lim_{x \to 0} \frac{1}{2x} \log\, [p^2(x) + q^2(x)] = c_1$, and thus

$$\lim_{\varepsilon \to 0} \frac{1}{2x} \log\left[p^2(x) + q^2(x)\right]\Big|_{-\varepsilon}^{\varepsilon} = c_1 - c_1 = 0 \ . \tag{3.6}$$

It is also easy to see that

$$\lim_{x \to \infty} \frac{1}{2x} \log\left[p^2(x) + q^2(x)\right] = 0 \ . \tag{3.7}$$

From (3.6) and (3.7) we have:

$$\begin{aligned} & \int_{D_M} \left[\frac{1}{2x} \log\left[p^2(x) + q^2(x)\right]\right]' dx \\ = \;& \frac{1}{2x} \log\left[p^2(x) + q^2(x)\right]\Big|_{-\infty}^{-1/M} + \frac{1}{2x} \log\left[p^2(x) + q^2(x)\right]\Big|_{1/M}^{+\infty} \\ = \;& -\frac{1}{2x} \log\left[p^2(x) + q^2(x)\right]\Big|_{-1/M}^{1/M} \to 0 \qquad (\text{when } M \to +\infty) \ . \end{aligned} \tag{3.8}$$

Finally, taking the real parts for both sides of (3.2) and substituting (3.3) and (3.8) into it, leads to:

$$\begin{aligned} \mathbb{E}_{re}(\phi) &= \frac{1}{\pi} \lim_{M \to +\infty} \int_{D_M} \mathrm{Re}\left[\frac{(g(x/i))'}{x\, g(x/i)}\right] dx \\ &= \frac{1}{\pi} \lim_{M \to +\infty} \int_{D_M} \left(\left[\frac{1}{2x} \log\left[p^2(x) + q^2(x)\right]\right]' + \frac{1}{2x^2} \log\left[p^2(x) + q^2(x)\right]\right) dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log\left[p^2(x) + q^2(x)\right] dx \ . \end{aligned} \tag{3.9}$$

This is what we call the real form of Coulson integral formula (for real energy of a complex polynomial), where the last integral in (3.9) should be understood as the principal value at $x = 0$.

Remark 1. In general, for the imaginary part of the energy $\mathbb{E}(\phi)$, we first note that

$$\frac{p(x)\,q'(x) - q(x)\,p'(x)}{p^2(x) + q^2(x)} = \left(arctg\frac{q(x)}{p(x)}\right)' .$$

So, similar to (3.3),

$$\begin{aligned} \mathrm{Im}\left[\frac{(g(x/i))'}{x\,g(x/i)}\right] &= \mathrm{Im}\left(\frac{p'(x) + iq'(x)}{x[p(x) + iq(x)]}\right) = \frac{p(x)\,q'(x) - q(x)\,p'(x)}{x[p^2(x) + q^2(x)]} \\ &= \left(\frac{1}{x}\ arctg\frac{q(x)}{p(x)}\right)' + \frac{1}{x^2}\ arctg\frac{q(x)}{p(x)} . \end{aligned}$$

From (3.4) and (3.5) it follows

$$\lim_{x\to 0}\frac{1}{x}\ arctg\frac{q(x)}{p(x)} = -b_1$$

and it is also obvious that

$$\lim_{x\to\infty}\frac{1}{x}\ arctg\frac{q(x)}{p(x)} = 0 .$$

So, similar to (3.8) we have

$$\begin{aligned} \int\limits_{D_M}\left(\frac{1}{x}\ arctg\frac{q(x)}{p(x)}\right)' dx &= \frac{1}{x}\ arctg\frac{q(x)}{p(x)}\bigg|_{-\infty}^{-1/M} + \frac{1}{x}\ arctg\frac{q(x)}{p(x)}\bigg|_{1/M}^{+\infty} \\ &= -\frac{1}{x}\ arctg\frac{q(x)}{p(x)}\bigg|_{-1/M}^{1/M} \longrightarrow b_1 - b_1 = 0 \quad (\text{when } M\to+\infty) . \end{aligned}$$

Thus from (3.2) we get:

$$\begin{aligned} \mathrm{Im}(\mathbb{E}(\phi)) &= \frac{1}{\pi}\lim_{M\to+\infty}\int\limits_{D_M}\mathrm{Im}\left[\frac{(g(x/i))'}{x\,g(x/i)}\right]dx \\ &= \frac{1}{\pi}\lim_{M\to+\infty}\int\limits_{D_M}\left(\frac{1}{x}\ arctg\frac{q(x)}{p(x)}\right)' dx + \frac{1}{\pi}\lim_{M\to+\infty}\int\limits_{D_M}\frac{1}{x^2}\ arctg\frac{q(x)}{p(x)}\,dx \\ &= \frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\frac{1}{x^2}\ arctg\frac{q(x)}{p(x)}\,dx \end{aligned} \tag{3.10}$$

where (same as in the case of (3.9)) the last integral in (3.10) should be understood as the principal value at $x = 0$.

Combining (3.9) and (3.10), we finally obtain:

Theorem 3.1. *Let* $\phi(z) = \sum_{k=0}^{n} a_k\, z^{n-k}$ *be a complex polynomial with* $a_0 = 1$ *and* $a_k = b_k + c_k\, i$, *where* b_k, c_k *are real numbers* $(k = 0, 1, \ldots, n)$. *Let the real polynomials* $p(x)$ *and* $q(x)$ *be defined as in (3.4) and (3.5). Then*

$$\mathbb{E}(\phi) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log\left[p^2(x) + q^2(x)\right] dx + \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2}\, arctg \frac{q(x)}{p(x)}\, dx\ .$$

Remark 2. If $\phi(z)$ is a real polynomial, then $p(x)$ and $q(x)$ have the following simple forms:

$$p(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, a_{2k}\, x^{2k} \quad , \quad q(x) = \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} (-1)^{k+1}\, a_{2k+1}\, x^{2k+1}\ . \tag{3.11}$$

Also in this case, $arctg[q(x)/p(x)]$ is an odd function, so (again) we have $\mathbb{E}(\phi) = \mathbb{E}_{re}(\phi)$ for real polynomials.

4 Some applications to the energies of digraphs

In [12], the energy of a digraph D is defined as

$$\mathbb{E}(D) = \sum_{k=1}^{n} |\operatorname{Re}(z_k)|$$

where $z_1, \ldots, z_n$ are the eigenvalues of the adjacency matrix $A(D)$ of D.

By (1.3), we see that $\mathbb{E}(D) = \mathbb{E}_{re}(\phi)$, where $\phi(x)$ is the characteristic polynomial of the adjacency matrix $A(D)$ of the digraph D. Since $\phi(x)$ is now a real polynomial, by the arguments in §1, we see that $\mathbb{E}(D) = \mathbb{E}_{re}(\phi) = \mathbb{E}(\phi)$.

In [12], Peña and Rada used a corollary of the complex form of Coulson integral formula to obtain an integral formula for the energy of a digraph D, all of whose cycles have length h, where $h \equiv 2 \pmod 4$. In that formula, all the terms inside the logarithm in the integrand have non-negative coefficients. But the corollary they used still contains the logarithm of some complex function.

In this section, we generalize their result to the digraphs in which every cycle has length an odd multiple of h, where $h \equiv 2 \pmod 4$ is a fixed positive integer. Furthermore, the approach we use to prove this generalization is to apply our real form (3.9) of the integral formula for energies. Thus we can avoid using the logarithm of a complex function in the proof of this generalization.

Let $\phi(x) = \sum_{k=0}^{n} a_k\, x^{n-k}$ be the characteristic polynomial of a digraph D. Then the well-known Sachs formula is [2]:

$$a_k = \sum_{L \in \mathcal{L}_k} (-1)^{comp(L)} \tag{4.1}$$

where $\mathcal{L}_k$ is the set of all linear subdigraphs of D with k vertices, and $comp(L)$ denotes the number of components of L.

Theorem 4.1. *Let $h \equiv 2 \pmod 4$ be a fixed positive integer, and $\phi(x) = \sum_{k=0}^{n} a_k\, x^{n-k}$ (where $a_0 = 1$) be a real polynomial of the following form:*

$$\phi(x) = \sum_{k=0}^{\lfloor n/h \rfloor} a_{hk}\, x^{n-hk}\ . \tag{4.2}$$

Note that $a_t \neq 0$ implies that t is a multiple of h. Then we have:

$$\mathbb{E}(\phi) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \log \left[\sum_{k=0}^{\lfloor n/h \rfloor} (-1)^k\, a_{hk}\, x^{hk} \right] \frac{dx}{x^2}\ . \tag{4.3}$$

Proof. Using formula (3.11), we have $q(x) = 0$ since h is even. This implies that all the coefficients a_{2k+1} are equal to zero.

On the other hand, if some $a_{2k} \neq 0$, then $h | 2k$, so there exists some integer t, such that $k = \frac{1}{2}\, ht$. Thus from (3.11) it follows:

$$p(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, a_{2k}\, x^{2k} = \sum_{t=0}^{\lfloor n/h \rfloor} (-1)^{\frac{1}{2}ht}\, a_{ht}\, x^{ht} = \sum_{t=0}^{\lfloor n/h \rfloor} (-1)^t\, a_{ht}\, x^{ht} \tag{4.4}$$

since $\frac{1}{2}\, h$ is an odd number.

Substituting (4.4) and $q(x) = 0$ into the real integral formula (3.9), we obtain (4.3). □

Lemma 4.1. *Let h be a positive integer and D be a digraph of order n. Let $\phi(x) = \phi_D(x) = \sum_{k=0}^{n} a_k\, x^{n-k}$ be the characteristic polynomial of D. Then $\phi(x)$ has the form (4.2) if and only if the length of every cycle of D is a multiple of h.*

Proof. Sufficiency: If $a_t \neq 0$, then $\mathcal{L}_t \neq \emptyset$ by the Sachs formula (4.1). Take $L \in \mathcal{L}_t$. Then t is the sum of the lengths of the cycles of L. Thus t is a multiple of h by hypothesis.

Necessity: Suppose to the contrary that the length of some cycle of D is not a multiple of h. Let t be the minimal such length. Then it can be verified that any linear subdigraph $L \in \mathcal{L}_t$ must consist of exactly one cycle (of length t). Thus we have

$$a_t = \sum_{L \in \mathcal{L}_t} (-1)^{comp(L)} = -c_t \neq 0$$

where c_t is the number of t-cycles of D, a contradiction. □

We now arrive at the following generalization of Theorem 5.3 from [12].

Theorem 4.2. *Let $h \equiv 2 \pmod 4$ be a fixed positive integer, and D be a digraph of order n each of whose cycles has length an odd multiple of h. Let $\phi(x) = \sum_{k=0}^{n} a_k \, x^{n-k}$ be the characteristic polynomial of D. Then we have:*
(1) $\mathbb{E}(D) = \mathbb{E}(\phi)$ has the from (4.3).
(2) $(-1)^k \, a_{hk} \geq 0$ for all $k = 0, 1, \ldots, \lfloor n/h \rfloor$.

Proof. The result (1) follows directly from Theorem 4.1 and Lemma 4.1.

For result (2), take any $L \in \mathcal{L}_{hk}$. Let $h\,c_1, \ldots, h\,c_r$ be the lengths of all the cycles of L. Then $c_1, \ldots, c_r$ are all odd and $c_1 + \cdots + c_r = k$. Thus we have

$$(-1)^{comp(L)} = (-1)^r = (-1)^{c_1 + \cdots + c_r} = (-1)^k \; .$$

This implies

$$a_{hk} = \sum_{L \in \mathcal{L}_{hk}} (-1)^{comp(L)} = (-1)^k \, |\mathcal{L}_{hk}| \; .$$

Thus $(-1)^k \, a_{hk} = |\mathcal{L}_{hk}| \geq 0$. □

Remark 3. From (4.3) and $(-1)^k \, a_{hk} \geq 0$, we see that $\mathbb{E}(D)$ is a strictly increasing function of those numbers $|a_{hk}|$.

Note: If we take $h = 2$, then the hypothesis in Theorem 4.2 can be restated as: The length of every cycle of D is even, but not a multiple of 4.

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